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ORIGINAL

Incorporation of Coupled Nonequilibrium Chemistry Into a Two-Dimensional Nozzle Code (SEAGULL)

Alan W. Ratliff

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Incorporation of Coupled Nonequilibrium Chemistry Into a Two-Dimensional Nozzle Code (SEAGULL)

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SUMMARY AND INTRODUCTION

During the past decade several excellent computer codes for analyses of complicated flow fields have been developed. NASA-Langley's SEAGULL program (Appendix A) that treats multiple shock waves and contact surfaces, using a floating shock fitting technique, is one such code. Previously, calculations performed with this code were limited to the ideal gas assumption. It is the purpose of this document to describe the extension of the code to handle real gas effects via the incorporation of a general finite rate chemistry and vibrational energy exchange package.

This document and the associated computer code (modified SEAGULL) now provide NASA-Langley with a benchmark finite rate general chemistry nozzle and plume code. The modified code retains all of its original features plus the capability to treat chemical and vibrational nonequilibrium chemistry. The chemistry package is extremely general in nature, handling any chemical reaction or vibrational energy exchange mechanism as long as thermodynamic data and rate constants are available for all participating species.

1. SYMBOLS

Symbol	Description
A	defined as used
b(z)	lower duct wall ordinate
c(z)	upper duct wall ordinate
C_p	specific heat at constant pressure
C_v	specific heat at constant volume
f(s)	entropy production (Eq. 4)
f_i	weighting factors (Eq. 15)
F_i	species mole/mass ratio
G	defined by Eq. (50)
h	static enthalpy
H	total enthalpy
k	reaction rate constant
K_p	equilibrium constant
P	natural log of pressure
p	pressure
q	total velocity
r	radial coordinate
$\mathfrak{R}$	universal gas constant
R	universal gas constant divided by global molecular weight

Symbol	Description
s	entropy
T	temperature
u	radial velocity component
w	axial velocity component
$\dot{w}_i$	net production rate of species i
X	transformed radial coordinate
y	axial coordinate
z	axial coordinate

Greek

α_i	species mole fraction
β	defined by Eq. (3)
γ	ratio of specific heats
ν_i', ν_i''	stoichiometric coefficients
ρ	density
ψ_i	species molecular weight
ψ	global molecular weight

Subscripts

i	refers to species i
in.	refers to initial conditions

2. DISCUSSION

2.1 BASELINE NOZZLE CODE – PROGRAM SEAGULL

Program SEAGULL is a computer code for the numerical analysis of complex two-dimensional or axisymmetric supersonic inviscid flows of a perfect gas. The fundamental limitation of this program is that the component of the Mach number in the axial direction at any point in the flow field must remain supersonic. The program was primarily designed for the analysis of internal flows. It can compute the flow field produced by a single duct or several ducts that are merged. Although designed for internal flows, it can also compute jets and plumes. The program continuously monitors the flow field to detect the formation of shock waves. All discontinuities are treated explicitly, and all interactions are treated by a locally exact solution. A description of the method used is given in Appendix A.

2.2 MODIFIED NOZZLE CODE

The modified program Seagull is now a computer code for the numerical analysis of complex two-dimensional or axisymmetric supersonic inviscid flows with fully coupled nonequilibrium chemistry. The code retains all the salient features discussed in Section 2.1, plus the additional capability to treat frozen or finite rate chemically reacting flows. The generalized chemistry package included in the modified Seagull also permits the analysis of vibrational nonequilibrium energy exchanges.

2.3 DEVELOPMENT OF EQUATIONS

The basic equations governing the flow of gases with nonequilibrium reacting chemistry are the following:

$$
\left.
\begin{aligned}
&\nabla \cdot \rho\bar{q} = 0 && \text{Global Continuity}\\
&\nabla\bar{q} \cdot \rho\bar{q} + \nabla p = 0 && \text{Momentum}\\
&\rho\bar{q} \cdot \nabla H = 0 && \text{Energy}\\
&\rho\bar{q} \cdot \nabla F_i - \dot{w}_i = 0 && \text{Species Continuity}\\
&p = \rho\, \Re T \sum_{i=1}^{N} \frac{\alpha_i}{\psi_i} && \text{Equation of State}\\
&H = h + \frac{1}{2}\nabla(\bar{q} \cdot \bar{q}) && \text{Total Enthalpy}\\
&\dot{w}_i = \frac{\rho}{\psi_i} \sum_{j=1}^{M} (\nu''_{i,j} - \nu'_{i,j}) \left[k_f \prod_{\ell=1}^{N} F_\ell^{\nu'_{\ell,j}} - k_b \prod_{\ell=1}^{N} F_\ell^{\nu'_{\ell,j}} \right] && \text{General Species Production Rate}
\end{aligned}
\right\} \quad (1)
$$

where N species are involved in M reactions.

These equations are expanded in a Cartesian coordinate system, scaled (i.e., nondimensionalized) with respect to some initial reference conditions, and are then solved in the modified SEAGULL code.

To avoid unnecessarily complicating the discussion, the remainder of the derivation is shown for a two-dimensional case only. The code, however, can also handle axisymmetrics flows.

Scaled and expanded, the equations then become

$$\left.\begin{aligned}
&\beta P_z + wu_r + A_1 wu P_r - uw_r - \frac{w}{A_2} f(s) = 0 \\
&\beta w_z + \frac{T}{\psi} u_r + A_1 wu w_r - A_1 \frac{T}{\psi} u P_r + \frac{T}{A_2 \psi} f(s) = 0 \\
&u_z + \frac{u}{w} u_r + \frac{T}{w\psi} P_r = 0 \\
&wF_{i_z} + uF_{i_r} - \frac{\dot{w}}{\rho} = 0 \\
&H_z + \frac{u}{w} H_r = 0
\end{aligned}\right\} \qquad (2)$$

where the subscripts refer to differentiation with respect to the r, z coordinates.

β, A_1 and A_2 are conveniently defined as follows:

$$\left.\begin{aligned}
\beta &= A_1 w^2 - \frac{T}{\psi} \\
A_1 &= 1 - \frac{\gamma_{in} - 1}{A_2} \\
A_2 &= \gamma_{in} C_p
\end{aligned}\right\} \qquad (3)$$

The function f(s) is the entropy production due to finite rate chemical reactions.

$$f(s) = (\bar{q} \cdot \nabla s)_{chem} \qquad (4)$$

The general set of governing equations (Eq. (2)) are then recast in terms of the computational coordinates (X, Z) that are defined by

$$X = (r - b(z))/(c(z) - b(z))$$

and (5)

$$Z = z$$

where b(z) and c(z) define the lower and upper walls of the duct or nozzle.

All the primary variables in the equation set are scaled with respect to the initial conditions. The pressure, density, temperature and molecular weight are non-dimensionalized by p_{in}, ρ_{in}, T_{in}, ψ_{in}, respectively. Velocity is conveniently scaled by $\sqrt{p_{in}/\rho_{in}}$ and entropy is non-dimensionalized by the specific heat at constant volume $C_{v_{in}}$, i.e., $S = ([S] - [S_{in}])/C_{v_{in}}$.

The specific heat at constant pressure, C_p, is scaled with respect to its initial value, $[C_p] = [C_p]/[C_{p_{in}}]$. Static enthalpy is non-dimensionalized by $C_{p_{in}} T_{in}$, and for consistency the total enthalpy equation then becomes

$$H_T = h + \frac{[\mathfrak{R}]}{[C_{p_{in}}]} (u^2 + w^2)\psi \qquad (6)$$

where all values are non-dimensional except $[\mathfrak{R}]$ and $[C_{p_{in}}]$.

The finite rate chemistry parameters, of course, have dimensional characteristics. Interrelationships between the flow field and the finite rate reactions are treated internally by temporarily dimensioning the variables appearing in the species continuity equations. The reacting chemistry calculation is then carried out and the results are subsequently non-dimensionalized.

2.4 SOLUTION TECHNIQUE

A finite difference numerical scheme utilizing the explicit MacCormack operator is used to integrate the equations for conservation of global mass, momentum and energy. The species conservation equations are solved by an implicit technique similar to that developed by Moretti (Ref. 1). This method was chosen to provide good stability characteristics in the overall numerical scheme.

The general solution technique is discussed adequately in Appendix A. The same methodology is retained in the modified SEAGULL with the finite rate reacting chemistry. The only exception is the species continuity equation set which is solved by the following technique.

A detailed description of the rate processes that occur in finite rate reacting flows requires that a myriad of mechanisms be considered to include all the possible chemical and vibrational reactions of dissociation, formation, recombination, etc.

All of these, however, can be treated with a very general formalism. In the form usually quoted in chemical kinetics (Ref. 2) the phenomenological law of mass action states that the rate of a reaction is proportional to the product of the concentrations of the reactants. Thus, for a general reaction of the form

$$\sum_{j=1}^{N} \nu'_j A_j \rightleftharpoons \sum_{j=1}^{N} \nu''_j A_j \tag{7}$$

the net rate of production $\dot{w}_i$ for any participating species for which the stoichiometric coefficients ν'_i and ν''_i are not equal can then be written as

$$\dot{w}_i = \frac{\rho}{\Psi_i} \sum_{j=1}^{M} (\nu''_{i,j} - \nu'_{i,j}) \left[k_f \prod_{\ell=1}^{N} F_\ell^{\nu'_{\ell,j}} k_b \prod_{\ell=1}^{N} F_\ell^{\nu''_{\ell,j}} \right] \tag{8}$$

Assuming small deviations from equilibrium, the forward and backward reaction rate constants, k_f and k_b, respectively, can be related to the concentration equilibrium constant and to the pressure equilibrium constant as follows:

$$\frac{k_f}{k_b} = K_c = K_p (\Re T)^{\sum_{i=1}^{N} (\nu'_i - \nu''_i)} \tag{9}$$

The significance of the pressure equilibrium constant K_p is that it can be easily evaluated for any reaction using tabulated values of K_f the equilibrium constant for formation from the elements. Values of K_f are commonly tabulated in conjunction with specific heats, entropies and enthalpies as a function of temperature, and are available in general for most species. An equally

convenient method exists for determining K_p from the change of free energy accompanying the reaction, i.e.,

$$K_p = \exp(-\Delta G/\Re T) \tag{10}$$

where ΔG is the change in free energy during the reaction process. Free energy values are also available for most species in tabular form. This method is used to compute K_p in Program SEAGULL. The JANNAF thermochemical tables (Ref. 4) are used as the source for obtaining input data for various chemical systems. ΔG is computed directly by taking the difference in free energy between the products and reactants.

For reasons of computational speed and efficiency, the program contains explicit expressions, as obtained from Eq. (11), for the most commonly encountered reaction mechanisms. Twelve types of reaction mechanisms are considered as possible contributors to the calculation of the net rate of production, $\dot{w}_i$.

Reaction Type				
(1, 7)	A + B	$\rightleftharpoons$	C + D	
(2, 8)	A + B + M	$\rightleftharpoons$	C + M	
(3, 9)	A + B	$\rightleftharpoons$	C + D + E	
(4, 10)	A + B	$\rightleftharpoons$	C	(11)
(5, 11)	A + M	$\rightleftharpoons$	C + D + M	
(6, 12)	A + M	$\rightleftharpoons$	C + M	

Reaction types (7) through (12) correspond to reaction types (1) through (6), but proceed in the forward direction only.

To reduce roundoff and truncation errors, the forward and backward rates for each reaction are computed separately. All contributions to the molar rate of production of a given species are then computed and added algebraically to form matrix coefficients (discussed later). Since reaction types (7) through (14) proceed in the forward direction only, the second term on the right-hand side of Eq. (11) is disregarded in calculating the contributions to the coefficient matrix.

In reactions (2), (5) and (6) as well as in (8), (11) and (12), M denotes a third body species which can be specified. For these reactions the situation often occurs where for various third bodies the respective rate constants differ only by a constant multiplier. These multipliers can be considered as third body efficiencies or weighting factors. If such a case is encountered, the third body species mole mass ratio F_M becomes effectively a fictitious mole mass ratio, consisting of the weighted sum over all those species having a nonzero weighting factor, i.e.,

$$F_M = \sum_i f_i F_{M_i} \tag{12}$$

where f_i are the weighting factors.

The forward rate constant, k_f, is generally a function of temperature. It is most often expressed in Arrhenius form. Again, for speed and efficiency in computation, the rate constants are divided into five types:

Rate Constant Type		
(1)	$k_f = A$	
(2)	$k_f = AT^{-N}$	
(3)	$k_f = A \exp(B/\Re T)$	(13)
(4)	$k_f = AT^{-N} \exp(B/\Re T)$	
(5)	$k_f = AT^{-N} \exp(B/\Re T^M)$	

The equations presented in this document provide a very general formalism for the evaluation of various rate processes. The specification of particular systems and associated rate constant will be up to the program user.

Consider now the general species continuity equation

$$\rho \bar{q} \cdot \nabla F_i = \dot{w}_i \tag{14}$$

and making use of the foregoing discussion of the rate process we now proceed to describe a calculational technique for determining the individual species composition on a point-by-point basis. The description of this process is substantially simplified if Eq. (11) is specialized to a particular reaction type, say number (7) from Eq. (14) which is a one-way, two-body reaction.

$$A + B \rightarrow C + D \tag{15}$$

the net production rate for this process is

$$\dot{w} = -k_f \rho^2 F_A F_B \tag{16}$$

and the species continuity equation for species B then becomes

$$\rho \bar{q} \cdot \nabla F_B = -k_f \rho^2 F_A F_B \tag{17}$$

This equation can readily be solved using finite difference techniques employing explicit relationships, such as Euler or more sophisticated schemes, such as Runge-Kutta. The step size for integrating this equation, however, is severely limited by stability criteria. It can be seen from Eq. (20) that the rate of change of a species along the streamline becomes increasingly larger as the flow speed is slowed, the density increased, or for fast reaction rates. In rocket engine problems, combinations of slow speeds, high densities and fast reaction rates (i.e., quasi-equilibrium) are quite common and integration step sizes so small (i.e., $< 10^{-8}$ meters) are encountered that the solution becomes impractical in terms of computation time.

For this reason, the technique described in Ref. 3 based on a linearization of the production rates was utilized. Writing Eq. (20) in finite difference form over an integration step from station n at $z = z_o$ to n+1 at $z = z_o + \Delta z$

$$F_{B_{n+1}} = F_{B_n} - \frac{k_f \Delta z \rho}{q} F_{A_{n+1}} F_{B_{n+1}} - \frac{u}{w} \Delta z \frac{\partial F_{B_n}}{\partial r} \tag{18}$$

And evaluating all the species concentrations at the downstream point results in a set of simultaneous nonlinear algebraic equations. The lateral gradient term $\frac{\partial F_B}{\partial r_n}$ is evaluated at the upstream station n and uses windward differences. In order to solve these equations we must then linearize the term $F_{A_{n+1}} F_{B_{n+}}$ which is accomplished following the lead of Ref. 3. If this term is expanded in terms of its values at station n along with the increments over n to n+1 we can obtain the following expression.

$$F_{A_{n+1}} F_{B_{n+1}} = F_{A_n} F_{B_{n+1}} + F_{B_n} F_{A_{n+1}} - F_{A_n} F_{B_n} \tag{19}$$

neglecting products of differentials which are assumed to be of second order importance. Equation (21) can now be written in its linearized form. Let $C = \Delta z \, k_f \rho / w$, then

$$F_{B_{n+1}} = F_{B_n} - C \left[F_{A_n} F_{B_{n+1}} + F_{B_n} F_{A_{n+1}} - F_{A_n} F_{B_n} \right] - \frac{u}{w} \Delta z \frac{\partial F_B}{\partial r_n}$$

and similarly, (20)

$$F_{A_{n+1}} = F_{A_n} - C \left[F_{A_{n+1}} F_{B_n} + F_{B_{n+1}} F_{A_n} - F_{A_n} F_{B_n} \right] - \frac{u}{w} \Delta z \frac{\partial F_A}{\partial r_n}$$

Equation (20) can then be expressed in terms of a set of unknowns and calculable coefficients, C. Rewriting these we obtain

$$\begin{aligned} F_{B_{n+1}} &= Q_{B_n} - C\,F_{A_n}\,(F_{B_{n+1}}) - C\,F_{B_n}\,(F_{A_{n+1}}) \\ F_{A_{n+1}} &= Q_{A_n} - C\,F_{B_n}\,(F_{A_{n+1}}) - C\,F_{A_n}\,(F_{B_{n+1}}) \end{aligned} \tag{21}$$

where

$$Q_{i_n} = F_{i_n} + C F_{i_n} F_{j_n} - \frac{u}{w}\,\Delta z\,\frac{\partial F_i}{\partial r_n} \tag{22}$$

$$\begin{aligned} F_{A_{n+1}}\,(1 + C\,F_{B_n}) + (C\,F_{A_n})\,F_{B_{n+1}} &= Q_{A_n} \\ F_{A_{n+1}}\,(C\,F_{B_n}) + (1 + C\,F_{A_n})\,F_{B_{n+1}} &= Q_{B_n} \end{aligned} \tag{23}$$

A matrix can now be formed using totally known information.

$$\begin{bmatrix} 1 + C\,F_{B_n} & C\,F_{A_n} \\ C\,F_{B_n} & 1 + C\,F_{A_n} \end{bmatrix} \begin{bmatrix} F_{A_{n+1}} \\ F_{B_{n+1}} \end{bmatrix} = \begin{bmatrix} Q_{A_n} \\ Q_{B_n} \end{bmatrix} \tag{24}$$

The matrix [A] [X] = [B] is then solved for the unknown compositions $F_{A_{n+1}}$, $F_{B_{n+1}}$ via a triangulation technique. Although consuming more time per integration step than an explicit formulation, the implicit technique employed here is unconditionally stable permitting much larger step sizes, thus allowing solutions to be obtained for problems where the small steps required by the explicit technique prevented even the consideration of the case. Finally it should be recalled that an extremely simple case was chosen only for purposes of illustration and the general technique coded in the modified Program SEAGULL will handle many species with multiple reactions.

2.5 BOUNDARY CONDITIONS

By combining the two momentum equations we obtain

$$\tau_z + w^2 \frac{\tau A_1}{\beta} \tau_r + \left(\frac{A_1 w^2 \tau^2}{\beta} + 1 \right) \frac{T}{\psi w^2} P_r - \frac{T}{\beta \psi} \frac{\tau}{w A_2} f(s) = 0 \qquad (25)$$

where $\tau = u/w$.

The global continuity equation is used in the form

$$P_z + \frac{w^2}{\beta} (\tau A_1 P_r + \tau_r) - \frac{w}{A_2 \beta} f(s) = 0 . \qquad (26)$$

Now, using Eqs. (28) and (29) that involve partials of P and τ only, a characteristics compatibility equation can be written

$$\frac{d\tau}{dz} \mp \frac{T}{w^2 \psi} \sqrt{\frac{A_1 (u^2 + w^2)}{T/\psi} - 1} \frac{dP}{dz} = RHS \qquad (27)$$

where the right-hand side (RHS) is:

$$RHS = \frac{f(s)}{A_2} \left[\frac{T}{\beta \psi w} \left(\tau \pm \sqrt{\frac{A_1 (u^2 + w^2)}{T/\psi} - 1} \right) \right] \qquad (28)$$

Then by combining these equations with the chain rule definitions,

$$\left.\begin{aligned} \frac{dP}{dz} &= \frac{\partial P}{\partial z} + \lambda \frac{\partial P}{\partial r} \\ \frac{d\tau}{dz} &= \frac{\partial \tau}{\partial z} + \lambda \frac{\partial \tau}{\partial r} \end{aligned}\right\} \qquad (29)$$

an equation for the axial pressure variation is obtained in terms of known quantities.

$$P_z = -\lambda P_r \mp \frac{w^2 (RHS - \tau_z - \lambda \tau_r)}{\frac{T}{\psi} \sqrt{\frac{A_1 (u^2 + w^2)}{T/\psi} - 1}} \qquad (30)$$

where

$$\lambda = \frac{w^2 \tau A_1}{\beta} \mp \frac{T}{\beta \psi} \sqrt{\frac{A_1 (u^2 + w^2)}{T/\psi} - 1} \tag{31}$$

By integrating Eq. (30), the pressure is obtained at the new wall point and the velocity is computed from the streamwise momentum equation

$$\rho q \frac{\partial q}{\partial s} = - \frac{\partial P}{\partial s} \tag{32}$$

Velocity components u and w are then obtained from the known wall slope. The boundary conditions are completed by integrating the species continuity equations along the wall in a manner similar to that used for the interior points.

2.6 SHOCK WAVES

The general scheme outlined in Appendix A is utilized for computing shock wave information. The original ideal gas analysis was supplemented by the addition of methodology to handle reacting gas calculations across the shocks.

Figure 1 illustrates a stream tube passing through an oblique shock wave. This wave, which is extremely thin, will cause an almost instantaneous rise in pressure and temperature. For some distance downstream of the shock wave (in a reacting gas) a non-equilibrium zone will exist followed by a return to chemical equilibrium. The following analysis discusses the fluid flow properties in such a way that the non-equilibrium process need not be specified in order to arrive at an exact solution for the gas properties. It is impossible to determine the location of the new equilibrium shock point location without a detailed description of the non-equilibrium reaction process. It will be assumed therefore that this zone is thin and that no significant errors are introduced by letting the downstream physical location lie on the upstream location.

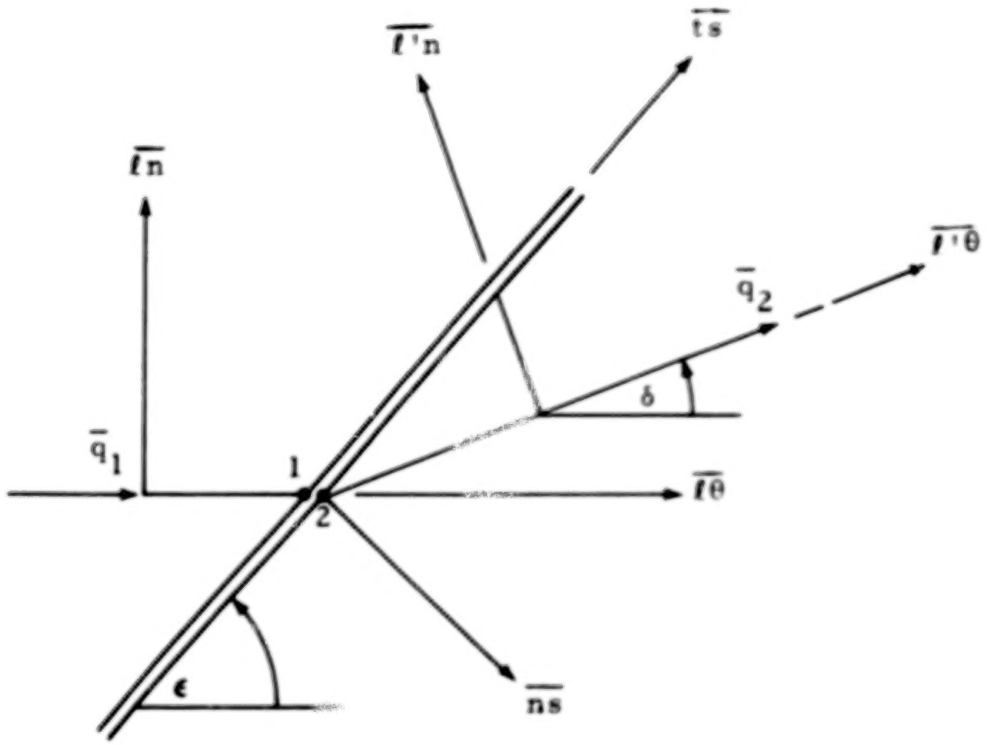
Consider a control surface as shown in the figure. The conservation of mass yields:

$$\rho_2 q_2 A_2 - \rho_1 q_1 A_1 = 0 \tag{33}$$

Let $\overline{ns}$ and $\overline{ts}$ be unit vectors normal and tangent to the shock surface, the unit vectors parallel and perpendicular to the streamline upstream of the shock are

$$\overline{\ell\theta} = \sin\epsilon\ \overline{ns} + \cos\epsilon\ \overline{ts}$$

$$\overline{\ell n} = -\cos\epsilon\ \overline{ns} + \sin\epsilon\ \overline{ts} \qquad (34)$$



and the unit vectors parallel and perpendicular to the streamline downstream of the shock are:

$$\overline{\ell\theta'} = \sin(\epsilon-\delta)\ \overline{ns} + \cos(\epsilon-\delta)\ \overline{ts}$$

$$\overline{\ell n'} = -\cos(\epsilon-\delta)\ \overline{ns} + \sin(\epsilon-\delta)\ \overline{ts} \qquad (35)$$

Conservation of momentum gives

$$-(p_1 + \rho_1 q_1^2) A_1 \overline{\ell\theta} + \frac{p_1 A_1}{\tan\epsilon} \overline{\ell n} + (p_2 + \rho_2 q_2^2) A_2 \overline{\ell\theta'} - \frac{p_2 A_2 \overline{\ell n}}{\tan(\epsilon - \delta)} \qquad (36)$$

and, after substitution of Eqs. (34) and (35) and setting each component to zero, Eq. (36) becomes,

$$\rho_2 q_2^2 \cos(\epsilon - \delta) A_2 - \rho_1 q_1^2 A_1 \cos\epsilon = 0 \qquad (37)$$

$$(p_1 + \rho_1 q_1^2) A_1 \sin\epsilon + \frac{p_1 A_1}{\tan\epsilon} \cos \quad - (p_2 + \rho_2 q_2^2) A_2 \sin(\epsilon - \delta)$$

$$- \frac{p_2 A_2 \cos(\epsilon - \delta)}{\tan(\epsilon - \theta)} = 0 \qquad (38)$$

But from geometry it can be seen that

$$\frac{A_2}{A_1} = \frac{\sin(\epsilon - \delta)}{\sin\epsilon} \qquad (39)$$

After substitution of Eqs. (40); (33), (37) and (38) become

$$\rho_2 q_2 \sin(\epsilon - \delta) - \rho_1 q_1 \sin\epsilon = 0 \qquad (40)$$

$$\rho_2 q_2^2 \sin(\epsilon-\delta)\cos(\epsilon-\delta) - \rho_1 q_1^2 \sin\epsilon\cos\epsilon = 0 \qquad (41)$$

$$p_2 + \rho_2 q_2^2 \sin^2(\epsilon-\delta) - p_1 - \rho_1 q_1^2 \sin^2\epsilon = 0 \qquad (42)$$

The above set of relations contains $\epsilon, \delta, p_2, \rho_2, q_2$ as unknown quantities, but

$$p_2 = p(s_2, q_2) \; ; \quad \rho_2 = \rho(s_2, q_2) \qquad (43)$$

So that if one variable, say ϵ, is taken as an independent parameter the remaining unknowns (δ, q_2, s_2) may be found by an iterative solution. These equations are, of course, formally the same as the ideal gas solution. The difference lies only in the variation of pressure etc., with entropy and velocity.

2.6.1 Iterative Solution of the Oblique Shock Relations

Rearranging Eq. (44) yields;

$$\sin(\epsilon - \delta) = \frac{\rho_1 q_1 \sin\epsilon}{\rho_2 q_2}$$

while squaring both sides of Eq. (45) and substituting the above relations yields, after simplification;

$$q_2 - q_1 \left\{ \left(\frac{\rho_1}{\rho_2}\right)^2 \sin^2\epsilon + \cos^2\epsilon \right\}^{1/2} = 0 \qquad (44)$$

and Eq. (42) becomes

$$p_2 + \rho_1 q_1^2 \sin^2\epsilon \left\{ \frac{\rho_1}{\rho_2} - 1 \right\} - p_1 = 0 \qquad (45)$$

In functional form Eqs. (44) and (45) are just

$$G_1(s_2, q_2) = 0$$

$$G_2(s_2, q_2) = 0 \tag{46}$$

From calculus

$$dG_1 = \frac{\partial G_1}{\partial q_2} dq_2 + \frac{\partial G_1}{\partial s_2} ds_2$$

$$dG_2 = \frac{\partial G_2}{\partial q_2} dq_2 + \frac{\partial G_2}{\partial s_2} ds_2 \tag{47}$$

Now

$$\left.\begin{aligned}
\frac{\partial G_1}{\partial q_2} &= 1 + q_1\left(\frac{q_1}{q_2}\right)\left(\frac{\rho_1}{\rho_2}\right)^2 \sin^2\epsilon \frac{\partial}{\partial q_2}\left(\ell n \rho_2\right) \\
\frac{\partial G_1}{\partial s_2} &= q_1\left(\frac{q_1}{q_2}\right)\left(\frac{\rho_1}{\rho_2}\right)^2 \sin^2\epsilon \frac{\partial}{\partial s_2}\left(\ell n \rho_2\right) \\
\frac{\partial G_2}{\partial q_2} &= p_2 \frac{\partial}{\partial q_2}\left(\ell n p_2\right) - \left(\frac{\rho_1}{\rho_2}\right)^2 q_1^2 \sin^2\epsilon\, \rho_2 \frac{\partial}{\partial q_2}\left(\ell n \rho_2\right) \\
\frac{\partial G_2}{\partial s_2} &= p_2 \frac{\partial}{\partial s_2}\left(\ell n p_2\right) - \left(\frac{\rho_1}{\rho_2}\right)^2 \sin^2\epsilon\, \rho_2 \frac{\partial}{\partial s_2}\left(\ell n \rho_2\right)
\end{aligned}\right\} \tag{48}$$

Rather than calculate the partial derivatives numerically by perturbing the functions $\ell n p_2$, $\ell n \rho_2$ approximate values for these derivaties will be found by assuming that locally the gas behaves ideally, that is to say

$$\frac{\partial R_2}{\partial s_2} = \frac{\partial R_2}{\partial q_2} = \frac{\partial \gamma_2}{\partial s_2} = \frac{\partial \gamma_2}{\partial q_2} = 0$$

so that holding q_2 constant

$$\frac{\partial(\ell n\, p_2)}{\partial s_2} \simeq \frac{\partial(\ell n\, \rho_2)}{\partial s_2} \simeq \frac{1}{1-\gamma_{in}} \tag{49}$$

and holding s_2 constant

$$\frac{\partial(\ell n\, p_2)}{\partial q_2} \simeq \gamma_2 \frac{\partial}{\partial q_2}(\ell n\, \rho_2) \simeq -\frac{q_2 \rho_2}{p_2} \tag{50}$$

writing Eq. (47) in finite difference form:*

$$G_1^{(n+1)} - G_1^{(n)} = \frac{\partial G_1^{(n)}}{\partial q_2}\left(q_2^{(n+1)} - q_2^{(n)}\right) + \frac{\partial G_1^{(n)}}{\partial s_2}\left(s_2^{(n+1)} - s_2^{(n)}\right)$$

$$G_2^{(n+1)} - G_2^{(n)} = \frac{\partial G_2^{(n)}}{\partial q_2}\left(q_2^{(n+1)} - q_2^{(n)}\right) + \frac{\partial G_2^{(n)}}{\partial s_2}\left(s_2^{(n+1)} - s_2^{(n)}\right)$$

Since the root $G_1 = G_2 = 0$ is desired, $G_1^{(n+1)}$, $G_2^{(n+1)}$ are set to zero, resulting in

---

*where n here is an iteration counter.

$$s^{(n+1)} = s^{(n)} + \left(G_2^{(n)} \frac{\partial G_1^{(n)}}{\partial q_2} - G_1^{(n)} \frac{\partial G_2^{(n)}}{\partial q_2} \right) \Bigg/$$

$$\left(\frac{\partial G_1^{(n)}}{\partial s_2} \frac{\partial G_2^{(n)}}{\partial q_2} - \frac{\partial G_2^{(n)}}{\partial s_2} \frac{\partial G_1^{(n)}}{\partial q_2} \right) \tag{51}$$

and

$$q_2^{(n+1)} = q_2^{(n)} - \left\{ G_1^{(n)} + \frac{\partial G_1^{(n)}}{\partial s_2} \left(s^{(n+1)} - s^{(n)} \right) \right\} \Bigg/ \frac{\partial G_1^{(n)}}{\partial q_2} \tag{52}$$

The iterative solution using Eqs. (51) and (52) is continued until the desired convergence of G_1 and G_2 is reached. The solution is completed by

$$\delta = \epsilon - \sin^{-1} \left\{ \frac{\rho_1 q_1}{\rho_2 q_2} \sin\epsilon \right\} \tag{53}$$

The first guess to start the solution is an ideal gas solution to the set of equations. If it is indeed an ideal gas under analysis the first guess is exact. These relations are

$$\delta = \epsilon - \tan^{-1} \left\{ \tan\epsilon \left(\frac{1}{M_1^2 \sin^2\epsilon} + \frac{\gamma_1 - 1}{2} \right) \frac{2}{\gamma_1 + 1} \right\}$$

$$q_2 = q_1 \frac{\cos\epsilon}{\cos(\epsilon - \delta)} \tag{54}$$

$$s_2 = s_1 + \frac{R_1}{\gamma_1 - 1} \left\{ \ell n \left[\frac{2\gamma_1 M_1^2 \sin^2\epsilon - (\gamma_1 - 1)}{\gamma_1 + 1} \right] + \gamma_1 \ell n \left[\frac{\tan(\epsilon - \delta)}{\tan\epsilon} \right] \right\}$$

2.7 CONTACT SURFACES

Contact surfaces or slip lines are computed utilizing the condition that the pressures and flow angles must match across the surface. The equations for pressure and flow angle developed for the wall boundary conditions are also applied at the contact surface except that the streamline slope must now be obtained iteratively utilizing the matching conditions. Equations (25) and (26) are transformed to the computational coordinates and integrated via the MacCormack operator as described in Appendix A. The predictor (first level) is applied to the high Mach number side of the slip line and the corrector (second level) is applied to the low Mach number side.

With the pressure and slope now known at the contact surface the velocity is again obtained from Eq. (35). The velocity components are then evaluated from the known slip line slope.

2.8 THERMODYNAMIC PROPERTIES

The modified Program SEAGULL handles general gases composed of various chemical species rather than a global gas. This requires thermodynamic data inputs for all participating species as well as for all vibrational levels of the various excited molecules involved in vibrational energy exchange. For these molecules it is assumed that the molecular rotation remains in equilibrium with the translational temperature but each molecule is allowed to vibrate independently, corresponding to the energy in its respective vibrational level.

Thermodynamic data are supplied to the code in the form of tabular inputs of specific heat, entropy and enthalpy for each species as a function of temperature and are taken directly from the JANAF thermochemical tables (Ref. 4).

2.9 VIBRATIONAL NONEQUILIBRIUM

To make maximum use of the current technology of finite rate formulations, the various vibrational levels of the respective excited molecules are treated as individual chemical species. In order to treat them as individual species, it is first assumed that the excited molecule can be resolved into its various vibrational levels each of which is then treated as a separate species. This assumption requires that the thermodynamic properties be separately specified for each vibrational level. It is further assumed that molecular rotation remains in equilibrium with the translational temperature but the molecules can vibrate independently of the translational temperature. Accordingly, each molecule is permitted to vibrate independently corresponding to the energy in its respective vibrational level.

Appendix A

SHOCK FITTING METHOD FOR COMPLICATED TWO-DIMENSIONAL SUPERSONIC FLOWS

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Shock Fitting Method for Complicated Two-Dimensional Supersonic Flows

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The floating shock fitting technique is examined. Second-order difference formulas are developed for the computation of discontinuities. A procedure is developed to compute mesh points that are crossed by discontinuities. The technique is applied to the calculation of internal two-dimensional flows with arbitrary number of shock waves and contact surfaces. A new procedure, based on the coalescence of characteristics, is developed to detect the formation of shock waves. Results are presented to validate and demonstrate the versatility of the technique.

I. Introduction

INVISCID supersonic flows are governed by a first-order quasi-linear hyperbolic system of equations. The numerical computation of these flows is complicated, because the regular solution may break down due to the nonlinearity of the governing equations. The breakdown is characterized by the appearance of surfaces, such as shock waves and vortex sheets, across which the dependent variables or their derivatives are discontinuous. During the last decade, 2 numerical techniques have emerged for the analysis of these flows. One, known as shock capturing, tries to remove the explicit computation of the discontinuities by generalizing the concept of a solution of the Euler equations to include weak solutions (i.e., discontinuities). Because the shock capturing scheme requires no special treatment to deal with discontinuties, it has become an extremely popular way of computing. However, despite its present popularity, the results obtained with this technique[1] force us to agree with Moretti's conclusion that shock capturing is a poor interpretation of a physical phenomenon, and an extremely uneconomical way of computing.[2]

The other technique, known as shock fitting, makes special provisions for explicitly computing the discontinuties. In essence, it locates the discontinuties and treats them as boundaries between regions where a regular solution is valid. The effectiveness and soundness of this approach has been proven for a large number of problems involving 2, 3, and 4 independent variables. However, for problems in 3 or more independent variables, the partitioning of a flowfield into regions where a regular solution is valid, can create some difficult topological problems.[3] Recently, Moretti[4] has developed a technique (reminiscent of that proposed by Richtmyer and Morton,[5] that treats the discontinuities explicitly but does not require them as boundaries of the flow. This therefore eliminates the problems associated with partitioning the flowfield. It is this technique, known as floating shock fitting, that forms the subject matter of this paper.

To avoid unnecessary complications, the technique will be discussed in the context of a two-dimensional problem. However, to demonstrate the capabilities of the technique, results from complex flowfields are presented.

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Index categories: Nozzle and Channel Flow; Shock Waves and Denotations; Supersonic and Hypersonic Flow.

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II. Problem Definition

We will discuss the floating shock fitting technique as it applies to the flow of an inviscid, perfect gas through a two-dimensional duct of arbitrary geometry. The flow is assumed to be supersonic throughout, and consequently, irregular shock reflections are not considered. Shock waves generated by either discontinuities in the slopes of the walls, or by coalescence of pressure waves, will be automatically detected and fitted into the calculation. The number of shock waves, contact surfaces, and the number of interactions of these discontinuities, is considered arbitrary (limited only by computer storage).

III. Governing Equations

The flow variables are nondimensionalized by scaling the pressure, density, and temperature, with respect to their initial values (p_i, ρ_i, T_i), scaling the velocities with respect to $(p_i/\rho_i)^{1/2}$, and scaling all lengths with respect to some arbitrary reference length. The Euler equations written in a Cartesian frame (r,z), with the z-axis running along the length of the duct, are

$$P_r + (uwP_z + \gamma w u_z - \gamma u w_z)/\beta = 0$$

$$w_r + (uww_z - \gamma T u_z - TuP_z)/\beta = 0$$

$$u_r + (uu_z + TP_z)/w = 0$$

$$S_r + uS_z/w = 0 \tag{1}$$

Where P is the natural logarithm of pressure, u and w are the velocity components in the r and z directions, respectively; S is the entropy, γ is the ratio of specific heats; the temperature is given by

$$T = \exp[(S + (\gamma - 1)P)/\gamma] \tag{2}$$

and $\beta = w^2 - \gamma T$.

The following equations are introduced here for later reference. By combining the 2 momentum equations, we get

$$\tau_z + \frac{w^2\tau\tau_r}{\beta} + \left(1 + \frac{\tau^2 w^2}{\beta}\right)\frac{TP_r}{w^2} = 0 \tag{3a}$$

where $\tau = u/w$. With Eq. (3a) and the continuity equation in the form

$$P_z + w^2(\tau P_r + \gamma\tau_r)/\beta = 0 \tag{3b}$$

we can obtain the compatibility equation

$$\tau' \pm ([\gamma T(\beta + w^2\tau^2)]^{1/2}/\gamma w^2)P' = 0 \tag{4}$$

where the primes denote differentiation along the characteristic directions

$$\lambda^* = (w^2\tau \pm [\gamma T(\beta + w^2\tau^2)]^{1/2})/\beta \tag{5}$$

The Euler Eqs. (1) are recast in terms of computational coordinates (X,Z) defined by

$$X = (r - b(z))/(c(z) - b(z)) \quad Z = z \tag{6}$$

where $r = b(z)$ and $r = c(z)$ define the lower and upper walls of the duct. In matrix form the equations of motion become

$$f_Z = \underline{A} f_X \tag{7}$$

where the vector f is

$$f = \begin{bmatrix} P \\ u \\ w \\ S \end{bmatrix} \tag{8}$$

and the matrix $\underline{A}$ is

$$\underline{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ a_{31} & a_{32} & a_{11} & 0 \\ 0 & 0 & 0 & a_{22} \end{bmatrix} \tag{9}$$

$$a_{11} = -(uwX_r + \beta X_z)/\beta$$

$$a_{12} = -\gamma w X_r/\beta$$

$$a_{13} = \gamma u X_r/\beta$$

$$a_{21} = -TX_r/w$$

$$a_{22} = -(uX_r + wX_z)/w$$

$$a_{31} = uTX_r/\beta$$

$$a_{32} = \gamma TX_r/\beta$$

IV. Interior Point Computation

Unlike shock fitting, floating shock fitting does not subdivide the computational plane into regions bounded by discontinuities; instead, a single region is used, as illustrated in Fig. 1. In this single region, mesh points are equally spaced, and all discontinuties are allowed to move freely or float over the fixed grid. Their motion is subject only to the governing equations.

Except for the mesh points at the walls and in the neighborhood of a discontinuity, all mesh points are computed using the MacCormack scheme[6] to integrate Eq. (7). For example, consider the section of a duct, in the computational plane, sketched in Fig. 1. Using the MacCormack scheme, and assuming the solution is known at the Kth steps, $f_{N,K+1}$ is obtained from

level 1

$$f_{N,K+1} = f_{N,K} + \underline{A}_{N,K}(f_{N+1,K} - f_{N,K})\Delta Z/\Delta X$$

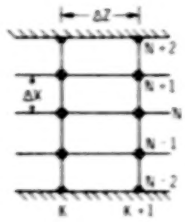

Fig. 1 Computational plane.

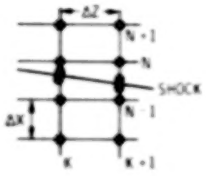

Fig. 2 Computation in the neighborhood of a shock wave.

level 2

$$f_{N,K+1} = \tfrac{1}{2}(f_{N,K} + f_{N,K+1} + \tilde{A}_{N,K+1}$$
$$(f_{N,K+1} - f_{N-1,K+1})\Delta Z/\Delta X) \tag{10}$$

Because the discontinuties are allowed to float over the fixed grid, special provisions must be taken when evaluating the X derivatives of f, at mesh points in the neighbornood of a discontinuity. Consider again the computation of point $(N,K+1)$, but now in the presence of a shock as shown in Fig. 2. There is no difficulty in computing the first level of the MacCormack scheme, since the forward difference

$$f_X = (f_{N+1,K} - f_{N,K})/\Delta X$$

is valid. However, for the second level, the backward difference

$$f_X = (f_{N,K+1} - f_{N-1,K+1})/\Delta X$$

is not allowed because f is not differentiable across the shock. On the other hand, the very simple approximation,

$$f_X = (f_{N,K+1} - f_{s,K+1})/(X_N - \hat{X}_{s,K+1})$$

where s denotes conditions at the shock, can result in large truncation errors, and the computation becomes unstable. Moretti recommends using an approximation that involves the values at the shock and the 3 neighboring mesh points [Eq. (61) in Ref. 2]. We have not used this approximation, because it makes the numerical domain of dependence point $(N,K+1)$ much larger than it physically is. Instead, we use the following approximation

$$f_X = -[(0.5\epsilon - 1)f_{N+1,K+1} + 0.5f_{s,K+1}$$
$$+ 0.5(1 - \epsilon)f_{N,K+1}]/\Delta X \tag{11}$$

where

$$\epsilon = (X_{N,K+1} - \hat{X}_{s,K+1})/\Delta X$$

The truncation error for Eq. (11), (based on f_X, not f) is given by

$$(\epsilon + 2)(\epsilon - 1)\Delta X/4 f_{XX}$$

With Eq. (11), the computation of point $(N,K+1)$ proceeds as the computation of any other interior point. Similar considerations apply to the computation of point $(N-1,K+1)$.

If point $(N+1, K+1)$ is not available when applying Eq. (11), as is the case indicated in Fig. 3 where 2 shocks are

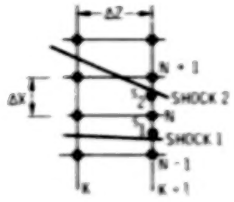

Fig. 3 Computation with closely spaced shocks.

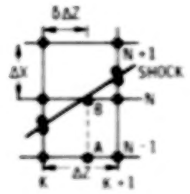

Fig. 4 Computation when a shock crosses a mesh line.

shown close to each other, then if the distance between the shocks is greater than ΔX, f_X is approximated by

$$f_X = (f_{\hat{2},K+1} - f_{\hat{1},K+1}) / (\hat{X}_{\hat{2},K+1} - \hat{X}_{\hat{1},K+1}) \tag{12}$$

If, however, the distance between the shocks is smaller than ΔX, the values at $(N,K+1)$ are interpolated from the shock values.

When a discontinuity crosses a mesh line, the computation of this mesh point must be modified. In Fig. 4, an up-running shock is shown crossing the Nth mesh line between steps K and $K+1$. The usual interior point computation would require taking the one-sided difference between points $(N+K, K)$ and (N,K) for level one. This procedure is no longer proper, because of the presence of the shock. We, therefore, proceed by evaluating points A and B as follows

$$\left.\begin{aligned} f_A &= F_{N-1,K} + \delta(\tilde{f}_{N-1,K+1} - f_{N-1,K}) \\ f_B &= f_{\hat{1},K} + \delta(\tilde{f}_{\hat{1},K+1} - f_{\hat{1},K}) \end{aligned}\right\} \tag{13}$$

where

$$\delta = (X_N - X_{\hat{1},K}) / (\hat{X}_{\hat{1},K+1} - X_{\hat{1},K}) \tag{14}$$

then, the value of f for level one at $(N, K+1)$ is

$$f_{N,K+1} = f_B + A_N (f_B - f_A)(1-\delta)\Delta Z / \Delta X \tag{15}$$

Care must be taken in evaluating δ when $dX_s/dZ \approx 0.$, since Eq. (14) becomes indeterminate. We therefore require that,

$$\left| \frac{dX_s}{dZ} \right| \Delta Z > 0.2 \Delta X$$

otherwise, δ is set to one to give the desired result

$$f_{N,K+1} = f_{\hat{1},K+1}$$

A similar computation is performed when a down-running discontinuity crosses a mesh line.

V. Wall Computation

The compatibility equation, Eq. (4), is applied at the wall to evaluate P_J

$$P_J = -\beta P_X + \frac{\gamma w^2}{[\gamma T(\beta + w^2\tau^2)]^{1/2}} (\tau_J + \lambda \tau_X) \tag{16}$$

where

$$\lambda = X_\zeta + \lambda^+ X_r$$

Here, the X derivatives are evaluated as three-point one-sided differences and

$$\tau_J = \begin{cases} b_{zz} \text{ for } \lambda^- \\ c_{zz} \text{ for } \lambda^+ \end{cases}$$

Then, following the MacCormack algorithm, the value of the pressure at the wall, P_w, is given by

$$\tilde{P}_{w,K+1} = P_{w,K} + P_J \Delta Z$$

$$P_{w,K+1} = \tfrac{1}{2}(P_{w,K} + \tilde{P}_{w,K+1} + \tilde{P}_J \Delta Z)$$

With the pressure and entropy known at the wall, the temperature is obtained from Eq. (2), and the magnitude of the velocity from

$$\frac{w^2 + w^2}{2} + \frac{\gamma}{\gamma - 1} T = \text{constant} \tag{17}$$

The two-velocity component can then be determined from the known wall slope and the vanishing of the velocity component normal to the wall.

VI. Shock Detection

Perhaps the most distinguishing feature of the problem we are considering, and certainly its most troublesome one, is the possible formation of shock waves. In this section, we will consider the procedure required to detect an incipient shock. There are two important features for any such procedure. First, the procedure must be reliable. Incipient shocks must be located at the proper place, but most important, the procedure must be able to interpret the physics of the problem accurately, and should not be so sensitive as to create nonexistent shocks. Secondly, because the procedure must be executed at every step, it must be very fast and require a minimum amount of data to make a reliable decision.

The procedure we have constructed, based on the concept of coalescing characteristics, requires only information on 2 adjacent mesh points, and we find it to be both reliable and fast. However, its empirical nature should be kept in mind. It is applied at the end of a computational step as follows:

Assume that the flowfield is known at the Kth step (see Fig. 5). At each mesh point N and $N-1$, the up-running $(\lambda_N^+, \lambda_{N-1}^+)$ and downrunning $(\lambda_N^-, \lambda_{N-1}^-)$ characteristics are evaluated using Eq. (5). If we now assume that the ΔZ intervals between steps (evaluated from the *CFL* condition)[6] are essentially the same, then a quantity η^*, which is the reciprocal of the number of steps needed for 2 characteristics to coalesce can be evaluated from

$$\eta^* = (\lambda_{N-1}^+ - \lambda_N^+) \Delta z / \Delta r$$

A considerable number of numerical experiments indicate that a shock should be fitted into the calculation when η^* becomes greater than 0.22 (approximately 4 steps before the characteristics coalesce).

We have found that for a wide range of problems, if the detection of incipient shocks is delayed until $\eta^* < 0.22$, then the procedure becomes very sensitive and shocks are predicted unnecessarily.

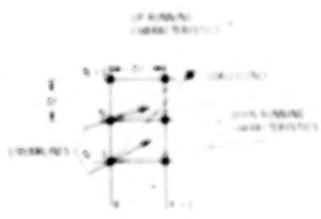

Fig. 5 Details of the shock detection.

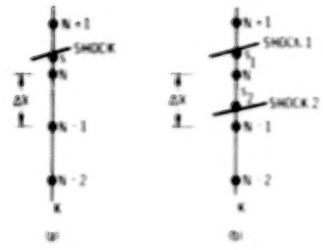

Fig. 6 Evaluation of the low-pressure side of a shock.

The detected shock is assumed to have the average slope of the coalescing characteristics and to be located half way between r_N and r_{N-2}. With the initial shock location known, the initial flowfield variables on the low pressure side are linearly interpolated between the 2 mesh points bracketing the shock, and on the high pressure side they are linearly extrapolated using the 2 mesh points next to the shock on the high pressure side.

Shocks that are generated at the walls of the duct, because of slope discontinuities at the walls, are introduced from user supplied information on the wall geometries, and do not make use of the procedure described in this section.

VII. Shock Computation

The low-pressure side of a shock is computed using the same scheme described for the interior point computation, but using the X derivatives given in this section. In Fig. 6, assuming that mesh point N lies on the low-pressure side, the X derivatives at the shock for the predictor level are evaluated from

$$f_{X_s} = \left[\frac{2}{1+\epsilon} (f_{s,A} - f_{N-1,A}) + 0.5 f_{N-2,A} - \frac{(0.5+\epsilon)}{(1+2\epsilon)} f_{N,A} \right] / \Delta X \tag{18}$$

where

$$\epsilon = (X_{s,A} - X_{N,A}) / \Delta X \tag{19}$$

If only two mesh points are available, then the derivatives are evaluated from

$$f_{X_s} = \left[\frac{2\epsilon - 1}{1+\epsilon} f_{N-1,A} + \frac{3}{1+\epsilon} f_{s,A} - 2 f_{N,A} \right] / \Delta X \tag{20}$$

with ϵ given by Eq. (19). The truncation error for Eq. (18) is of order ΔX^2 and for Eq. (20) it is

$$(\epsilon - 1) \frac{\Delta X}{2} f_{XX_s}$$

It should be noted that Eqs. (18-20) are not the same formulas suggested by Moretti,[2,4] particularly Eq. (18) has a lower truncation error than Moretti's counterpart.

If only 1 mesh point is available (Fig. 6b), then f_{X_s} is approximated by

$$f_{X_s} = (f_{s1,A} - f_{s2,A}) / (X_{s1,A} - X_{s2,A}) \tag{21}$$

provided that $(X_{s1,A} - X_{s2,A})$ is greater than ΔX. If $(X_{s1,A} - X_{s2,A})$ is smaller than ΔX, then f_{X_s} is set to zero. For the corrector stage, the same derivatives are used but with f replaced by $\bar{f}$.

If the low-pressure side lies on the other side of the shock, the derivatives that are used are the negatives of those given by Eq. (18) and Eq. (20), and ϵ is given by the negative of Eq. (19).

The computation of the high-pressure side of the shock has been formulated using the compatibility equation, Eq. (4), on the characteristic reaching the shock on the high-pressure side along with Rankine-Hugoniot conditions. The details of this classical treatment of the shock can be found in Ref. 4.

The computation of the high-pressure side was the only computation requiring involved programing logic. The main difficulty is the determination of the origin of the characteristic reaching the shock in the immediate vicinity of other discontinuities. It should be, however, possible to avoid these difficulties by computing the high-pressure side with the method suggested by Kentzer.[7]

VIII. Contact Surface Computation†

To compute a contact surface, we exploit the fact that both pressure and streamline slope are continuous across a contact surface. Eqs. (3a, b), which involve derivatives of P and τ only, are thus recast in terms of the computational coordinates (X,Z), and are integrated using the MacCormack scheme where the X derivatives are evaluated using Eq. (20). In the predictor level, Eq. (20) is applied on the high Mach number side of the contact surface. In the corrector level, it is applied on the low Mach number side. This choice is arbitrary, and the same results are obtained if the order is reversed.

With the pressure and entropy known at the contact surface, the magnitude of the velocity follows from Eq. (17), and the 2 velocity components can be determined from the evaluated streamline slope.

IX. Interactions

The interactions of the discontinuities with the walls of the duct and with each other are computed by locally exact solutions. The details of these calculations can be found in most text books in fluid mechanics, for example, Ref. 8, and will not be discussed here.

X. Elimination of Weak Discontinuity

Discontinuities with a Mach number difference across the discontinity of less than 1% are automatically eliminated from the computation. This feature is not a requirement of the technique. It has, however, been incorporated, because for most practical applications, tracing these weak discontinuties is not necessary. It speeds up the computation, and it avoids computing degenerate discontinuities (i.e. the contact surface formed by the interaction of 2 shock waves of equal strength).

XI. Results

The results of several calculations performed with the floating shock fitting technique are presented to demonstrate the accuracy and versatility of the technique. All the computations were done on a CDC 6600 computer. The core required to run the code is under 55000$_8$ locations.

The flowfield produced by a uniform flow impinging on a wedge is often used to validate numerical calculations. The problem is a trivial one, consisting of uniform properties in front and behind the shock wave. The exact solution for a freestream Mach number of 3.50 which is initially compressed by a 15° wedge and then expanded, such as to exactly cancel the shock wave generated by the wedge, is shown in Fig. 7. In the figure, the lower wall pressure distribution shown corresponds to the case where the expansion occurs a very short distance before the shock reflects from the wall. The exact solution is obtained with the floating shock fitting

†We have recently experienced some difficulties with this procedure when the contact surface is next to a strong expansion fan. The problems have been overcome by reformulating the contact surface computation along the guide lines discussed on the shock computation.

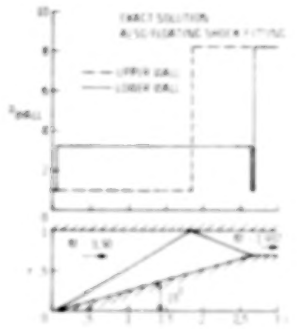

Fig. 7 Flowfield over a 15° wedge with shock cancellation.

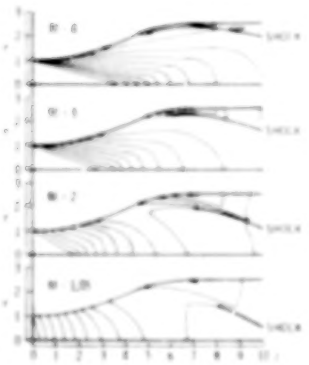

Fig. 8 Parametric study of a nozzle, showing shock waves and isobars.

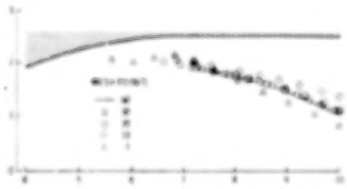

Fig. 9 Shock path for $M = 1$ case.

technique using only 2 mesh points in less than 1 sec of computational time (the same results are obtained increasing the number of mesh points).

In Fig. 8, the results of a parametric study of the flowfield produced by a nozzle are presented. The initial Mach number was used as the parameter, allowing it to range from near 1 to 4. Both the isobars and shock-wave patterns are shown in the figure. For the Mach 4 case, most of the isobars downstream of the shock wave were not included in the figure to avoid overcrowding of lines. The total computational time for these 4 cases, using 30 mesh points, was approximately 25 sec. Figures 9 and 10 give some further details in the calculation of the Mach 2 case. In these 2 figures the results obtained with 5, 10, 20, 30, and 60 points are shown. Figure 9 shows the calculated shock-wave path, while Fig. 10 shows the upper wall pressure distribution. The results show that a good qualitative result for this more complicated problem can be obtained with as few as 5 mesh points, and that good quantitative results are obtained with only 10 mesh points.

It is very often argued that shock fitting is limited in its capability to handle flowfields with more than a single shock.[9-11] In Refs. 3 and 12 this has been shown not to be the case for very complex three-dimensional steady, and one-dimensional time-dependent flows. We hope to fill the existing gap for two-dimensional steady problems with Fig. 11 and also to demonstrate that floating shock fitting is a numerically stable technique even in multishocked flowfields. In Fig. 11, the geometry of NASA Langley's scramjet combustor model is simulated. The results shown are for a flow with an incoming Mach number equal to 3, inclined at 8° with the horizontal. The resulting flowfield con-

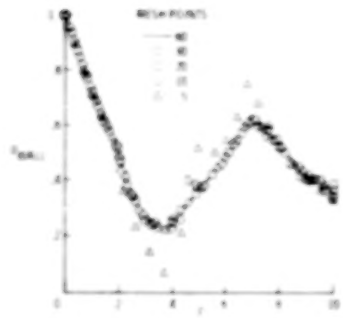

Fig. 10 Upper wall pressure for $M = 2$ case.

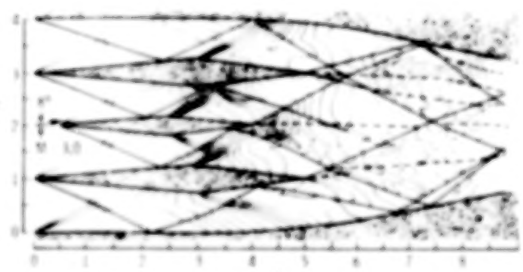

Fig. 11 Flowfield for a simulated scramjet, showing shock waves, vortex sheets and isobars.

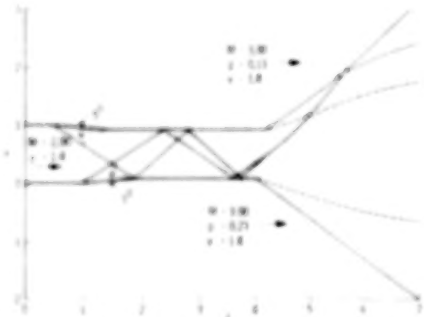

Fig. 12 Plume flowfield showing shock waves and vortex sheets.

sists of a complex pattern of interacting expansions and shock waves. In the figure, the shock-wave pattern is shown by the heavy lines. The contact surfaces are shown by the dashed lines, and isobars are shown by the light lines. Certain discontinuities are seen to terminate abruptly in the flowfield, while some shock interactions do not show the expected vortex sheet; this is a result of the automatic elimination of weak discontinuities previously discussed. The calculation was performed in 6 pieces, using a total of 120 mesh points and requiring approximately 2.2 min of computational time. The calculation shows approximately a dozen discontinuities, with some 40 interactions.

The technique has been extended to internal axisymmetric flows (with and without swirl), internal line source type flows, and to external two-dimensional flows. An example of the application to external flows is shown in Fig. 12, where a flow with an initial Mach number of 2.0 exhausts into a Mach 3.0 freestream. The lower wall ends at $z = 4.0$, while the upper wall ends at $z = 4.2$. The freestream conditions for the external flows are shown in the figure.

XII. Conclusions

Floating shock fitting for two-dimensional steady flows is an accurate and stable technique capable of solving very complex problems with acceptable running times. A fully three-dimensional code is planned for the near future.

References

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Appendix B

INPUT GUIDE AND SAMPLE CASES

Appendix B

INPUT GUIDE AND SAMPLE CASES

DESCRIPTION OF INPUT DATA

ALL INPUT DATA IS READ FROM TAPE 5.

*THE FIRST INPUT CARD CONSISTS OF 11 INTEGERS.
THE FORMAT IS 1615
THESE INTEGERS ARE ID, KOUT, ICN, IBN, ISO, NA, ISY, JJ, ITY, ITP, IVI
ITY IS USED TO INDICATE MERGING OF INTERNAL DUCTS, AND IS NOT RELATED TO JETS OR PLUMES.

ID=0 INPUT CARD NO. 3 IS NOT READ
ID=1 INPUT CARD NO. 3 IS READ
KOUT = THE NO. OF STEPS TAKEN BEFORE A COMPLETE OUTPUT OF THE FLOW FIELD IS MADE
ICN = THE TOTAL NO. OF SHARP CORNERS ON THE UPPER WALL
ICN CANNOT EXCEED 10
IBN = THE TOTAL NO. OF SHARP CORNERS ON THE LOWER WALL
IBN CANNOT EXCEED 10
ISO=0 NO ISOBAR OUTPUT WILL BE PROVIDED
ISO=1 ISOBARS WILL BE COMPUTED AND PRINTED AT EVERY STEP
NA = INITIAL NUMBER OF MESH POINTS MINUS TWO
NA CANNOT EXCEED 98
IN MOST CASES 20 POINTS ARE SUFFICIENT, AND ON THE AVERAGE THERE SHOULD BE ABOUT 5 POINTS BETWEEN DISCONTINUITIES.
ISY=0 NO SYMMETRY IS ASSUMED IN THE COMPUTATION OF THE LOWER WALL
ISY=1 SYMMETRY IS IMPOSED IN THE COMPUTATION OF THE LOWER WALL
JJ=0 FOR TWO DIMENSIONAL FLOW
JJ=1 FOR AXISYMMETRIC FLOW
JJ=2 FOR LINE SOURCE FLOW
ITY=0 A SINGLE DUCT CALCULATION
ITY=1 SINGLE DUCT CALCULATION WITH DATA WRITTEN ON TAPE 7 FOR FUTURE MERGING RUN. CAN ALSO BE USED TO RESTART A CALCULATION
ITY=2 DATA IS READ TO MERGE TWO OR MORE FLOWS, AND DATA IS WRITTEN ON TAPE 7 FOR FUTURE CONTINUATION
ITY=3 DATA IS READ TO MERGE TWO OR MORE FLOWS
ITP=0 NO CALCOMP PLOT IS GENERATED
ITP=1 A CALCOMP PLOT IS GENERATED
IVI=0 NO VISCOUS FORCES ARE COMPUTED
IVI=1 SPALDING-CHI USED TO COMPUTE VISCOUS FORCES, THE REYNOLDS NO. WILL BE BASED ON THE WALL GEOMETRY LENGTH

*INPUT CARD NO. 2 CONSISTS OF 5 INTEGERS
THE FORMAT IS 1615
NS = NO. OF CHEMICAL SPECIES
NT = NO. OF POINTS IN THERMODYNAMIC TABLES
NM = NO. OF CATALYTIC SPECIES
NR = NO. OF REACTIONS IN MECHANISM
IFROZE=0, FINITE RATE
IFROZE=1, FROZEN FLOW

*INPUT CARD NO. 3 IS READ ONLY IF ID=1
ITS PURPOSE IS SOLELY FOR IDENTIFICATION, A FREE FIELD FORMAT
IS USED BETWEEN COLUMNS 6 THRU 55

*INPUT CARD NO. 4 CONSISTS OF 5 FLOATING POINT NUMBERS
THE FORMAT IS 8E10.4
THESE NUMBERS ARE ACH, GM, DIST, TOLER, SCALE

ACH = INITIAL MACH NUMBER
GM = RATIO OF SPECIFIC HEATS
DIST = DISTANCE TO THE END OF THE CALCULATION (CM)
TOLER = A TOLERANCE PARAMETER TO INCREASE OR DECREASE THE NO. OF MESH POINTS. IT WORKS AS FOLLOWS: IF SET TO X THEN THE NO. OF MESH POINTS WILL BE INCREASED WHEN THE DISTANCE BETWEEN MESH POINTS IS X TIMES THE INITIAL DISTANCE BETWEEN MESH POINTS, AND MESH POINTS ARE DECREASED WHEN THE DISTANCE BETWEEN MESH POINTS IS 1./X TIMES THE INITIAL DISTANCE BETWEEN MESH POINTS. SETTING TOLER TO A LARGE NUMBER (SAY 1000.) HAS THE EFFECT OF NOT CHANGING THE NUMBER OF MESH POINTS.
SCALE = IS A SCALE FACTOR FOR CALCOMP PLOTS NEEDED ONLY IF ITP=1 BOTH THE R AND Z COORDINATES ARE MULTIPLIED BY SCALE BEFORE THEY ARE PLOTTED.

*INPUT CARD NO. 5 CONSISTS OF 7 FLOATING POINT NUMBERS
THE FORMAT IS 8E10.4
THE NUMBERS ARE ZEXIT, PINF, TINF, GMINF, ACHINF, ANGINF, RCINF
THIS INFORMATION IS NEEDED IN CASE THE LOWER WALL OF THE DUCT OPENS TO THE FREE STREAM AT Z=ZEXIT. IF THIS IS NOT THE CASE THEN ZEXIT SHOULD BE SET TO A NUMBER GREATER THAN THE VALUE OF DIST, AND THE REMAINING SIX NUMBERS NEED NOT BE DEFINED.

ZEXIT = LOCATION OF EXIT PLANE (CM)
PINF = FREE STREAM STATIC PRESSURE (ATM)
TINF = FREE STREAM STATIC TEMPERATURE ($^{\circ}$K)
GMINF = NOT REQUIRED PRESENTLY
ACHINF = FREE STREAM MACH NUMBER
ANGINF = FREE STREAM INCLINATION IN DEGREES, MEASURED POSITIVE COUNTERCLOCKWISE FROM THE Z AXIS
RCINF = NOT REQUIRED PRESENTLY

*INPUT CARD NO. 6 (REQUIRED ONLY IF ZEXIT. LE. DIST)
THE FORMAT IS 8E10.4
THIS CARD SUPPLIES THE SPECIES DISTRIBUTION IN THE EXTERNAL STREAM IN THE SAME ORDER AS IN THE MAIN STREAM*

ALFA(1, 1), FIRST SPECIES IN THERMO DATA TABLES
ALFA(2, 1), SECOND SPECIES IN THERMO DATA TABLES
ALFA(N, 1), N-TH SPECIES IN THERMO DATA TABLES

*INPUT CARD NO. 7 IS THE SAME AS CARD NO. 5, BUT FOR THE CASE WHEN THE UPPER WALL OF THE DUCT OPENS TO FREE STREAM.

*INPUT CARD NO. 8 IS THE SAME AS CARD NO. 6 BUT FOR THE CASE WHEN THE UPPER WALL OF THE DUCT OPENS TO FREE STREAM.

*INPUT CARD NO. 9 CONSISTS OF ICN FLOATING POINT NUMBERS, IF ICN=0 THE INPUT CARD IS NOT NEEDED. THESE NUMBERS ARE STORED IN ARRAY ZIC(N).
THE FORMAT IS 8E10.4

ZIC(N) = LOCATION OF THE NTH CORNER ON THE UPPER WALL (CM)

*INPUT CARD NO. 10 CONSISTS OF ICN FLOATING POINT NUMBERS, IF ICN=0 THE INPUT CARD IS NOT NEEDED' THESE NUMBERS ARE STORED IN ARRAY AIC(N).
THE FORMAT IS 8E10.4

AIC(N) = THE CHANGE IN ANGLE IN DEGREES AT THE NTH UPPER WALL CORNER. AIC IS DEFINED POSITIVE IF THE CORNER IS A COMPRESSION AND NEGATIVE IF AN EXPANSION. NOTE THAT IT IS A CHANGE IN ANGLE AND NOT THE NEW WALL ANGLE.

*INPUT CARD NO. 11 IS THE SAME AS CARD NO. 6, BUT FOR THE LOWER WALL. THE DATA IS STORED IN ARRAY ZIB(N), THE INPUT CARD IS NOT NEEDED IF IBN=0.

*INPUT CARD NO. 12 IS THE SAME AS CARD NO. 7, BUT FOR THE LOWER WALL. THE DATA IS STORED IN ARRAY AIB(N), THE INPUT CARD IS NOT NEEDED IF IBN=0. AIB IS DEFINED IN THE SAME WAY AS AIC.

*INPUT CARD NO. 13 CONSISTS OF 6 FLOATING POINT NUMBERS
THIS CARD IS NOT NEEDED IF IVI=0
THE FORMAT IS 8E10.4

ATWTI(1) = NONDIMENSIONAL LOWER WALL TEMPERATURE
ATWTI(2) = NONDIMENSIONAL UPPER WALL TEMPERATURE
XL(1) = LOWER WALL VIRTUAL ORIGIN FOR SPALDING-CHI (GREATER THAN 0.)
XL(2) = UPPER WALL VIRTUAL ORIGIN FOR SPALDING-CHI (GREATER THAN 0.)
REI = REYNOLDS NO. PER UNIT LENGTH
PRAND = PRANDTL NO.

---

*IF PARTICULAR SPECIES DOES NOT EXIST ENTER ZERO IN THAT LOCATION.

*INPUT CARD NO. 14 INITIAL PRESSURE AND TEMPERATURE IN INTERNAL DUCT.
THE FORMAT IS 8E10.4

PIN = INITIAL PRESSURE (ATM)
TIN = INITIAL TEMPERATURE (^{o}K)

*INPUT CARD(S) NO. 15 SPECIES DISTRIBUTION MOLE FRACTION IN INTERNAL DUCT.

ALFA(1, 1), FIRST SPECIES IN THERMO DATA TABLES
ALFA(2, 1), SECOND SPECIES IN THERMO DATA TABLES
ALFA(N, 1), NTH SPECIES IN THERMO DATA TABLES

*INPUT CARD(S) NO. 16 SPECIES ID AND THERMODYNAMIC DATA
THE FORMAT IS A6, 2E10.3

AID(I), ITH SPECIES IDENTIFICATION
WTM(I), ITH SPECIES MOLECULAR WEIGHT (g/g-mole)
HF(I), ITH SPECIES HEAT OF FORMATION (K-cal/mole)
TTB(J), JTH TEMPERATURE POINT IN TABLES (K)
CPTB(I, J) SPECIFIC HEAT FOR ITH SPECIES AT JTH TEMPERATURE POINT (cal/mole-K)
STB(K, J) ENTROPY FOR ITH SPECIES AT JTH TEMPERATURE POINT (cal/mole-K)
HTB(I, J) ENTHALPY FOR ITH SPECIES AT JTH TEMPERATURE POINT (K-cal/mole)

*INPUT CARD(S) NO. 17 CATALYTIC SPECIES DATA (OPTIONAL) INPUT ONLY IF NM=0
THE FORMAT IS A6/(16E5.2)
IF NM $\neq$ 0, INPUT THE FOLLOWING
AID(J), NAME OF JTH CATALYTIC SPECIES
WF(J, K), WEIGHTING FACTOR OF ITH SPECIES FOR JTH CATALYTIC SPECIES

AID(J), NAME OF JTH CATALYTIC SPECIES
WF(J, I), WEIGHTING FACTOR OF ITH SPECIES FOR JTH CATALYTIC SPECIES

*INPUT CARD NO. 18 NAME OF REACTION SET
THE FORMAT IS 13A6, A2

*INPUT CARD NO. 19 REACTION RATE DATA (OPTIONAL) INPUT ONLY IF IFROZE IS ZERO
THE FORMAT IS A6, 1X, A6, 1X, A6, 1X, A6, 1X, A6, 1X, A6, 7X, I2, I1, E8.2, F5.2, F10.1, 1F6.2

AID(J), SPECIES (NAME) APPEARING IN ITH REACTION
IRR(I), REACTION TYPE
IRT(I), RATE CONSTANT TYPE
RCT(I, N), RATE CONSTANT COEFFICIENTS N = 1, 4*

FOR MOST RUNS, WITH THE EXCEPTION OF CASES WHERE ITY=2 OR ITY=3, THIS IS ALL THE INFORMATION REQUIRED AS INPUT DATA. CASES WHERE ITY=2 OR ITY=3 WILL BE DISCUSSED LATER. LET US CONSIDER NOW THE DEFINITION OF THE WALL GEOMETRIES.

THE LOWER WALL GEOMETRY SHOULD BE DEFINED IN SUBROUTINE GEOMB. THE USER DEFINES THE GEOMETRY BY GIVING R OF THE WALL AS A FUNCTION OF THE AXIAL COORDINATE Z. THE CODE ASSUMES THAT THE INITIAL STATION IS AT Z=0. IF IT IS NECESSARY TO START THE CALCULATION AT SOME OTHER VALUE OF Z, THIS CAN BE DONE BY REDEFINING Z IN THE MAIN PROGRAM. IN ADDITION THE FIRST DERIVATIVE, RZ, AND THE SECOND DERIVATIVE, RZZ, ARE ALSO REQUIRED.

THE UPPER WALL GEOMETRY SHOULD BE DEFINED IN SUBROUTINE GEOMC. THE GEOMETRY IS DEFINED IN THE SAME MANNER AS DESCRIBED ABOVE. A SAMPLE UPPER GEOMETRY FOR A DUCT WITH AN INITIAL HEIGHT OF ONE UNIT, A 10. DEGREE COMPRESSION AT Z= .5 AND A 6 DEGREE EXPANSION AT Z=1. IS:

```
R=1.  $ RZ=0.  $ RZZ=0.  $ IF (Z.LT.0.5) RETURN
R=1. -.17633*(Z-.5)  $  RZ= -.17633  $ RZZ=0.
IF (Z.LT.1.) RETURN
R=.911835+.1051*(Z-1.)  $ RZ=.1051  $ RZZ=0.  $ RETURN
```

CARE SHOULD BE EXERCISED WHEN DEFINING WALL GEOMETRIES, AS THE MOST FREQUENT CAUSE OF PROBLEMS THAT USERS HAVE EXPERIENCED WITH THIS PROGRAM IS USUALLY RELATED TO IMPROPER GEOMETRY DEFINITION.

---

*The pre-exponential factor, N = 1, has units of (cm-particle-sec). The activation energy, N = 3, has the units (cal/mol).

SAMPLE CASE FOR FINITE RATE CHEMISTRY

```
@ELT,DIL DATA
ELT037 RLIB70 03/17-17:00:57-(,0)
000001      000   @XQT SEAGULL
000002      000        1    1    1    1    0   19
000003      000        7   20    3   14    0
000004      000          TWO DIMENSIONAL TEST CASE WITH SHOCK + INTERACTION
000005      000   6.0          1.23          9.0          10.0          3.0
000006      000   10.
000007      000   10.
000008      000   1.5
000009      000   *20.0
000010      000   1.0
000011      000   10.0
000012      000   .6805      1000.0
000013      000   .03497     .23927     .69388     2.47  -03 .02646     2.94  -03 0.0
000014      000   H          1.008      52.102
000015      000      200.          4.968     27.423      0.009     400.          4.968     28.852      0.506
000016      000      500.          4.968     29.961      1.003     600.          4.968     30.867      1.5
000017      000      700.          4.968     31.632      1.998     800.          4.968     32.296      2.493
000018      000      900.          4.968     32.881      2.990     1000.         4.968     33.404      3.487
000019      000     1200.          4.968     34.310      4.481     1400.         4.968     35.075      5.474
000020      000     1600.          4.968     35.739      6.468     1800.         4.968     36.325      7.461
000021      000     2000.          4.968     36.848      8.455     2200.         4.968     37.322      9.449
000022      000     2400.          4.968     37.754     10.442     2600.         4.968     38.152     11.436
000023      000     2800.          4.968     38.520     12.430     3000.         4.968     38.862     13.423
000024      000     3200.          4.968     39.183     14.417     3400.         4.968     39.484     15.410
000025      000   H2         2.016      0.0
000026      000      200.          6.894     31.251       .013     400.          6.975     33.247       .707
000027      000      500.          6.993     34.806      1.406     600.          7.009     36.082      2.106
000028      000      700.          7.036     37.165      2.808     800.          7.087     38.107      3.514
000029      000      900.          7.148     38.998      4.226     1000.         7.219     39.702      4.944
000030      000     1200.          7.390     41.033      6.404     1400.         7.600     42.187      7.902
000031      000     1600.          7.823     43.217      9.446     1800.         8.016     44.150     11.030
000032      000     2000.          8.195     45.004     12.651     2200.         8.358     45.793     14.307
000033      000     2400.          8.506     46.527     15.993     2600.         8.639     47.213     17.708
000034      000     2800.          8.757     47.857     19.448     3000.         8.859     48.465     21.210
000035      000     3200.          8.982     49.040     22.992     3400.         9.063     49.586     24.794
000036      000   H2O        18.016     -57.798
000037      000      200.          8.027     45.155      0.015     400.          8.186     47.484      0.825
000038      000      500.          8.415     49.334      1.654     600.          8.676     50.891      2.509
000039      000      700.          8.954     52.249      3.390     800.          9.246     53.469      4.300
000040      000      900.          9.547     54.570      5.240     1000.         9.851     55.592      6.209
000041      000     1200.         10.444     57.441      8.240     1400.        10.987     59.092     10.384
000042      000     1600.         11.462     60.591     12.630     1800.        11.869     61.965     14.964
000043      000     2000.         12.214     63.234     17.373     2200.        12.505     64.412     19.486
000044      000     2400.         12.753     65.511     22.372     2600.        12.965     66.541     24.945
000045      000     2800.         13.146     67.508     27.556     3000.        13.304     68.421     30.201
000046      000     3200.         13.441     69.284     32.876     3400.        13.562     70.102     35.577
000047      000   O          16.000     99.559
000048      000      200.          5.235     38.501      0.010     400.          5.135     39.991      0.528
000049      000      500.          5.081     41.131      1.038     600.          5.049     42.059      1.544
000050      000      700.          5.029     42.831      2.048     800.          5.015     43.501      2.550
000051      000      900.          5.006     44.092      3.052     1000.         4.999     44.619      3.552
000052      000     1200.          4.990     45.529      4.551     1400.         4.984     46.298      5.548
000053      000     1600.          4.981     46.963      6.544     1800.         4.979     47.590      7.540
000054      000     2000.          4.978     48.074      8.536     2200.         4.979     48.549      9.532
000055      000     2400.          4.981     48.982     10.527     2600.         4.986     49.381     11.524
000056      000     2800.          4.994     49.751     12.522     3000.         5.004     50.096     13.522
000057      000     3200.          5.017     50.419     14.524     3400.         5.033     50.724     15.529
```

```
000058  000  OH      17.0074     9.432
000059  000     200.          7.165     43.925     0.013    400.        7.087     45.974     2.725
000060  000     500.          7.055     47.551     1.432    600.        7.057     48.837     2.137
000061  000     700.          7.090     49.927     2.845    800.        7.150     50.877     3.556
000062  000     900.          7.233     51.724     4.275   1000.        7.332     52.491     5.003
000063  000    1200.          7.549     53.847     6.491   1400.        7.766     55.027     8.023
000064  000    1600.          7.963     56.077     9.596   1800.        8.137     57.025    11.207
000065  000    2000.          8.286     57.891    12.849   2200.        8.415     58.686    13.681
000066  000    2400.          8.526     59.424    16.214   2600.        8.622     60.110    17.929
000067  000    2800.          8.706     60.752    19.662   3000.        8.780     61.355    21.411
000068  000    3200.          8.846     61.924    23.174   3400.        8.905     62.462    24.949
000069  000  O2      31.9988     0.0
000070  000     200.          7.023     49.047     0.013    400.        7.196     51.091     2.724
000071  000     500.          7.431     52.722     1.455    600.        7.670     54.098     2.210
000072  000     700.          7.883     55.297     2.988    800.        8.063     56.361     3.786
000073  000     900.          8.212     57.320     4.600   1000.        8.336     58.192     5.427
000074  000    1200.          8.527     59.729     7.114   1400.        8.674     61.055     8.835
000075  000    1600.          8.800     62.722    10.583   1800.        8.916     63.265    12.354
000076  000    2000.          9.029     64.710    14.149   2200.        9.139     65.075    15.966
000077  000    2400.          9.248     65.876    17.804   2600.        9.354     66.620    19.664
000078  000    2800.          9.455     67.317    21.545   3000.        9.551     67.973    23.446
000079  000    3200.          9.640     68.592    25.365   3400.        9.723     69.179    27.302
0000e0  000  H02     33.008     5.0
0000e1  000     200.          8.347     54.434     0.015    400.        8.967     56.910     2.877
0000e2  000     500.          9.479     58.960     1.797    600.        9.980     60.734     3.771
0000e3  000     700.         10.405     62.305     3.791    800.       10.769     63.719     4.850
0000e4  000     900.         11.067     65.006     5.943   1000.       11.365     66.189     7.066
0000e5  000    1200.         11.831     68.304     9.387   1400.       12.197     70.156    11.791
0000e6  000    1600.         12.485     71.804    14.761   1800.       12.714     73.288    16.782
0000e7  000    2000.         12.895     74.638    19.343   2200.       13.041     75.874    21.937
0000e8  000    2400.         13.160     77.714    24.558   2600.       13.256     78.371    27.200
0000e9  000    2800.         13.336     79.057    29.859   3000.       13.403     79.979    32.534
0000f0  000    3200.0        13.50      65.0      35.0     3600.0      13.6       90.0      36.0
0000f1  000  M1
0000f2  000  1.0  1.0  6.0  1.0  1.0  1.0  1.0  1.0
0000f3  000  M2
0000f4  000  20.  2.5  10.  1.0  1.0  1.0  1.0  1.0
0000f5  000  M3
0000f6  000  1.0  2.5  16.  1.0  1.0  1.0  1.0  1.0
0000f7  000     H2 - O2 COMBUSTION KINETICS
0000f8  000  H     +H      +M2     =H2     +M2                    22 2.8E-30 1.0       0.0
0000f9  000  H     +O      +M1     =OH     +M1                    21 1.00-32 0.0       0.0
0000100 000  H     +OH     +M1     =H2O    +M1                    22 6.1E-26 2.0       0.0
0000101 000  H     +O2     +M3     =HO2    +M3                    23 5.5 -33          1000.0
0000102 000  O     +O      +M1     =O2     +M1                    24 3.8E-30 1.0    -340.0
0000103 000  OH    +H              =H2     +O                     14 1.4E-14-1.0    -7000.0
0000104 000  OH    +O              =H      +O2                    11 4.0E-11 0.0       0.0
0000105 000  OH    +H2             =H2O    +H                     14 1.0E-17-2.0    -2900.0
0000106 000  OH    +OH             =H2O    +O                     13 1.0E-11 0.0    -1100.0
0000107 000  HO2   +H              =H2     +O2                    13 4.2 -11        -  700.0
0000108 000  HO2   +H              =OH     +OH                    13 4.2 -10        -  1900.0
0000109 000  HO2   +H2             =H2O    +OH                    13 1.2 -12        - 10700.0
000110  000  HO2   +O              =OH     +O2                    13 8.0 -11        -  1000.0
000111  000  HO2   +OH             =H2O    +O2                    13 8.3 -11        -  1900.0

END OF DATA.


@ADD,P DATA

@XQT SEAGULL
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.....................................
.                                   .
.          PROGRAM SEAGULL          .
. SUPERSONIC INVISCID FLOW ANALYSIS .
.    NASA LANGLEY RESEARCH CENTER   .
.         RELEASED 02/01/76         .
.     LAST MODIFICATION 02/25/77    .
.                                   .
.....................................
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TWO DIMENSIONAL FLOW
 TWO DIMENSIONAL TEST CASE WITH SHOCK +  INTERACTI
OUTPUT AT EVERY      1 STEPS
GAMMA=    .1230+01 DISTANCE=    .9000+01 TOLERANCE=    .1000+02 SCALE=    .3000+01
ICN= 1  IBN= 1  ISO= 0  ISY= 0  ITY= 0  ITP= 0  IVI= 0
   .2000+02 DEGREES BREAK IN THE UPPER WALL AT Z=    .1500+01
   .1000+02 DEGREES BREAK IN THE LOWER WALL AT Z=    .1000+01
```

INITIAL CONDITIONS

TEMPERATURE(DEG. KELVIN)		1.0000000+03
VELOCITY (M/S)		5.3167825+03
PRESSURE(ATM)		6.8050000-01
DENSITY(G/CC)		1.1281265-04
MOLECULAR WT.		1.3602172+01
GAMMA		1.2846758+00
TOTAL ENTHALPY		5.7722905+11
ENTROPY		2.1301588+09
MOLE FRACTION	H	3.4969999-02
MOLE FRACTION	H2	2.3927000-01
MOLE FRACTION	H20	6.9387999-01
MOLE FRACTION	O	2.4700000-03
MOLE FRACTION	OH	2.6460000-02
MOLE FRACTION	O2	2.9400000-03
MOLE FRACTION	HO2	0.0000000

FINITE RATE CHEMISTRY CALCULATIONS

H2 - O2 C ONRUST ION KI METICS

REACTIONS BEING CONSIDERED

RF=A*EXP(B/RTOOM)/TOOM

								A	N	B	M
1	H	+ H	+ M2	= H2	+ M2		2 2	1.816+18	1.00	.0	.00
2	H	+ O	+ M1	= OH	+ M1		2 1	1.628+15	.00	.0	.00
3	H	+ OH	+ M1	= H20	+ M1		2 2	2.213+22	2.00	.0	.00
4	H	+ O2	+ M3	= HO2	+ M3		2 3	1.995+15	.00	1000.0	.00
5	O	+ O	+ M1	= O2	+ M1		2 4	1.379+18	1.00	-340.0	.00
6	OH	+ H		= H2	+ O		1 4	8.432+09	-1.00	-7000.0	.00
7	OH	+ O		= H	+ O2		1 1	2.409+15	.00	.0	.00
8	OH	+ H2		= H20	+ H		1 4	6.023+06	-2.00	-2900.0	.00
9	OH	+ OH		= H20	+ O		1 3	6.023+12	.00	-1180.0	.00
10	HO2	+ H		= H2	+ O2		1 3	2.530+13	.00	-700.0	.00
11	HO2	+ H		= OH	+ OH		1 3	2.530+14	.00	-1900.0	.00
12	HO2	+ H2		= H20	+ OH		1 3	7.228+11	.00	-18700.0	.00
13	HO2	+ O		= OH	+ O2		1 3	6.819+13	.00	-1000.0	.00
14	HO2	+ OH		= H20	+ O2		1 3	6.999+13	.00	-1000.0	.00

CATALYTIC SPECIES BEING CONSIDERED

M1 = 1.00 H , 1.00 H2 , 6.00 H20 , 1.00 O , 1.00 OH , 1.00 O2 , 1.00 HO2 ,

M2 =20.00 H , 2.50 H2 ,10.00 H20 , 1.00 O , 1.00 OH , 1.00 O2 , 1.00 HO2 ,

M3 = 1.00 H , 2.50 H2 ,16.00 H20 , 1.00 O , 1.00 OH , 1.00 O2 , 1.00 HO2 ,

R= 1 Z= .9000+00 OZ= .0000

LOWER WALL FORCES FR= .0000 FZ= .0000 M= .0000 VFR= .0000 VFZ= .0000 VM= .0000
UPPER WALL FORCES FR= .0000 FZ= .0000 M= .0000 VFR= .0000 VFZ= .0000 VM= .0000
SUM OF FORCES .0000 .0000 .0000 .0000 .0000 .0000
FORCE ON COMPUTATIONAL PLANE= .0000 AREA= .0000
MOMENT ABOUT Y AXIS= .0000 MOMENT ABOUT Z AXIS= .0000

I	N	W	P	U	R	T	S	V	TWE	RHO	HTOT
C	21	.1000+01	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	20	.9979+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	19	.8947+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	18	.8421+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	17	.7895+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	16	.7368+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	15	.6842+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	14	.6316+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	13	.5789+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	12	.5263+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	11	.4737+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	10	.4211+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01
C	9	.3684+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6000+01	.0000	.1000+01	.1538+01

0	8	.3158+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6800+01	.0000	.1000+01	.1538+01
0	7	.2632+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6800+01	.0000	.1000+01	.1538+01
0	6	.2106+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6800+01	.0000	.1000+01	.1538+01
0	5	.1579+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6800+01	.0000	.1000+01	.1538+01
0	4	.1053+00	.1000+01	.0000	.6801+01	.1000+01	.0000	.6800+01	.0000	.1000+01	.1538+01
0	3	.5263-01	.1000+01	.0000	.6801+01	.1000+01	.0000	.6800+01	.0000	.1000+01	.1538+01
0	2	.0000	.1000+01	.0000	.6801+01	.1000+01	.0000	.6800+01	.0000	.1000+01	.1538+01

MOLE FRACTIONS

PT	P(N)	H	H2	H2O	O	OH	O2	HO2	MOL WT	GAMMA
21	1.00000	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
20	.94737	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
19	.89474	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
18	.84211	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
17	.78947	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
16	.73684	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
15	.68421	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
14	.63158	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
13	.57895	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
12	.52632	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
11	.47368	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
10	.42105	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
9	.36842	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
8	.31579	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
7	.26316	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
6	.21053	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
5	.15789	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
4	.10526	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
3	.05263	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00
2	.00000	3.49704-02	2.39272-01	6.93887-01	2.47002-03	2.64601-02	2.94003-01	0.00000	9.9999D-01	1.28467+00

SAMPLE CASE FOR VIBRATIONAL NON-EQUILIBRIUM

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@ELT,DIL DATA
ELTOO7 RLI670 12/01-19:12:01-(,0)
000001      000   @XQT SEAGULL
000002      000       1  100    1    1   0  19
000003      000      12   24    4   20   0
000004      000          CCCC    0000   C A S E ***
000005      000   4.0        1.2        +30.0      10.0       3.0
000006      000   434.
000007      000   434.
000008      000   1.0
000009      000   -30.0
000010      000   0.998
000011      000   -3.2
000012      000   2.0        2000.      9340.
000013      000   0.00322  0.00162   0.00876   0.01083   0.01018   0.00873   0.00393
000014      000   0.37433  0.07024   0.05909   0.02363   0.42544
000015      000   C02100   44.01     -90.081
000016      000        0.          6.955     37.932    -2.074     50.          6.955     37.932    -1.725
000017      000      100.          6.955     42.753    -1.378    150.          6.955     45.574    -1.030
000018      000      200.          6.955     47.575    -0.682    250.          6.955     49.127    -0.334
000019      000      300.          6.955     50.395     0.013    400.          6.955     52.396     0.709
000020      000      500.          6.955     53.948     1.404    600.          6.955     55.216     2.100
000021      000      700.          6.955     56.288     2.796    800.          6.955     57.217     3.491
000022      000      900.          6.955     58.036     4.187   1000.          6.955     58.769     4.882
000023      000     1200.          6.955     60.037     6.273   1400.          6.955     61.109     7.664
000024      000     1600.          6.955     62.038     9.055   1800.          6.955     62.857    10.446
000025      000     2000.          6.955     63.590    11.838   2200.          6.955     64.253    13.229
000026      000     2400.          6.955     64.858    14.620   2600.          6.955     65.415    16.011
000027      000     2800.          6.955     65.930    17.402   3000.          6.955     66.410    18.793
000028      000   C02001   44.01     -87.331
000029      000        0.          6.955     37.932    -2.074     50.          6.955     37.932    -1.725
000030      000      100.          6.955     42.753    -1.378    150.          6.955     45.574    -1.030
000031      000      200.          6.955     47.575    -0.682    250.          6.955     49.127    -0.334
000032      000      300.          6.955     50.395     0.013    400.          6.955     52.396     0.709
000033      000      500.          6.955     53.948     1.404    600.          6.955     55.216     2.100
000034      000      700.          6.955     56.288     2.796    800.          6.955     57.217     3.491
000035      000      900.          6.955     58.036     4.187   1000.          6.955     58.769     4.882
000036      000     1200.          6.955     60.037     6.273   1400.          6.955     61.109     7.664
000037      000     1600.          6.955     62.038     9.055   1800.          6.955     62.857    10.446
000038      000     2000.          6.955     63.590    11.838   2200.          6.955     64.253    13.229
000039      000     2400.          6.955     64.858    14.620   2600.          6.955     65.415    16.011
000040      000     2800.          6.955     65.930    17.402   3000.          6.955     66.410    18.793
000041      000   C02000   44.01     -94.051
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000042    000        0.          6.955    37.932    -2.074     50.        6.955    37.932    -1.725
000043    000      100.          6.955    42.753    -1.378    150.        6.955    45.574    -1.030
000044    000      200.          6.955    47.575    -0.682    250.        6.955    49.127    -0.334
000045    000      300.          6.955    50.395     0.013    400.        6.955    52.396     0.709
000046    000      500.          6.955    53.948     1.404    600.        6.955    55.216     2.100
000047    000      700.          6.955    56.266     2.796    800.        6.955    57.217     3.491
000048    000      900.          6.955    58.036     4.187   1000.        6.955    58.769     4.882
000049    000     1200.          6.955    60.037     6.273   1400.        6.955    61.109     7.664
000050    000     1600.          6.955    62.038     9.055   1800.        6.955    62.857    10.446
000051    000     2000.          6.955    63.590    11.838   2200.        6.955    64.253    13.229
000052    000     2400.          6.955    64.856    14.620   2600.        6.955    65.415    16.011
000053    000     2800.          6.955    65.930    17.402   3000.        6.955    66.410    18.793
000054    000  C02110  44.01     -88.111
000055    000        0.          6.955    39.31     -2.074     50.        6.955    39.31     -1.725
000056    000      100.          6.955    44.131    -1.378    150.        6.955    46.951    -1.030
000057    000      200.          6.955    48.952    -0.682    250.        6.955    50.504    -0.334
000058    000      300.          6.955    51.772     0.013    400.        6.955    53.773     0.709
000059    000      500.          6.955    55.325     1.404    600.        6.955    56.593     2.100
000060    000      700.          6.955    57.665     2.796    800.        6.955    58.594     3.491
000061    000      900.          6.955    59.413     4.187   1000.        6.955    60.146     4.882
000062    000     1200.          6.955    61.414     6.273   1400.        6.955    62.487     7.664
000063    000     1600.          6.955    63.415     9.055   1800.        6.955    64.235    10.446
000064    000     2000.          6.955    64.967    11.838   2200.        6.955    65.63     13.229
000065    000     2400.          6.955    66.235    14.620   2600.        6.955    66.792    16.011
000066    000     2800.          6.955    67.308    17.402   3000.        6.955    67.788    18.793
000067    000  C02010  44.01     -92.141
000068    000        0.          6.955    39.31     -2.074     50.        6.955    39.31     -1.725
000069    000      100.          6.955    44.131    -1.378    150.        6.955    46.951    -1.030
000070    000      200.          6.955    48.952    -0.682    250.        6.955    50.504    -0.334
000071    000      300.          6.955    51.772     0.013    400.        6.955    53.773     0.709
000072    000      500.          6.955    55.325     1.404    600.        6.955    56.593     2.100
000073    000      700.          6.955    57.665     2.796    800.        6.955    58.594     3.491
000074    000      900.          6.955    59.413     4.187   1000.        6.955    60.146     4.882
000075    000     1200.          6.955    61.414     6.273   1400.        6.955    62.487     7.664
000076    000     1600.          6.955    63.415     9.055   1800.        6.955    64.235    10.446
000077    000     2000.          6.955    64.967    11.838   2200.        6.955    65.63     13.229
000078    000     2400.          6.955    66.235    14.620   2600.        6.955    66.792    16.011
000079    000     2800.0         6.955    67.308    17.402   3000.0       6.955    67.788    18.793
000080    000  C02020  44.01     -90.284
000081    000        0.          6.955    40.115    -2.074     50.        6.955    40.115    -1.725
000082    000      100.          6.955    44.936    -1.378    150.        6.955    47.757    -1.030
000083    000      200.          6.955    49.758    -0.682    250.        6.955    51.310    -0.334
000084    000      300.          6.955    52.578     0.013    400.        6.955    54.579     0.709
000085    000      500.          6.955    56.131     1.404    600.        6.955    57.399     2.100
000086    000      700.          6.955    58.471     2.796    800.        6.955    59.400     3.491
000087    000      900.          6.955    60.219     4.187   1000.        6.955    60.952     4.882
000088    000     1200.          6.955    62.220     6.273   1400.        6.955    63.292     7.664
000089    000     1600.          6.955    64.221     9.055   1800.        6.955    64.040    10.446
000090    000     2000.          6.955    65.773    11.838   2200.        6.955    66.436    13.229
000091    000     2400.          6.955    66.041    14.620   2600.        6.955    67.598    16.011
000092    000     2800.          6.955    68.113    17.402   3000.        6.955    68.593    18.793
000093    000  C02030  44.01     -88.531
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000094	000	0.		6.955	40.687	-2.074	50.	6.955	40.687	-1.725
000095	000	100.		6.955	45.508	-1.378	150.	6.955	48.329	-1.030
000096	000	200.		6.955	50.329	-0.682	250.	6.955	51.882	-0.334
000097	000	300.		6.955	53.150	0.013	400.	6.955	55.151	0.709
000098	000	500.		6.955	56.703	1.404	600.	6.955	57.971	2.100
000099	000	700.		6.955	59.043	2.796	800.	6.955	59.972	3.491
000100	000	900.		6.955	60.791	4.187	1000.	6.955	61.524	4.882
000101	000	1200.		6.955	62.792	6.273	1400.	6.955	63.664	7.664
000102	000	1600.		6.955	64.793	9.055	1800.	6.955	65.612	10.446
000103	000	2000.		6.955	66.345	11.838	2200.	6.955	67.008	13.229
000104	000	2400.		6.955	67.613	14.620	2600.	6.955	68.170	16.011
000105	000	2800.		6.955	68.685	17.402	3000.	6.955	69.165	18.793
000106	000	N2(0)	28.016	0.0	3.798	71.4				
000107	000	0.		6.955	33.339	-2.075	50.	6.955	33.339	-1.727
000108	000	100.		6.956	38.160	-1.379	150.	6.956	40.981	-1.031
000109	000	200.		6.957	42.982	-0.683	250.	6.957	44.535	-0.335
000110	000	300.		6.958	45.803	0.013	400.	6.959	47.805	0.709
000111	000	500.		6.960	49.357	1.405	600.	6.962	50.627	2.101
000112	000	700.		6.965	51.700	2.797	800.	6.968	52.631	3.494
000113	000	900.		6.972	53.451	4.190	1000.	6.975	54.186	4.888
000114	000	1200.		6.983	55.458	6.284	1400.	6.991	56.535	7.681
000115	000	1600.		6.999	57.470	8.963	1800.	7.008	58.294	10.481
000116	000	2000.		7.015	59.033	11.883	2200.	7.022	59.702	13.287
000117	000	2400.		7.031	60.313	14.692	2600.	7.038	60.876	16.099
000118	000	2800.		7.045	61.399	17.507	3000.	7.052	61.885	18.917
000119	000	N2(1)	28.016	6.655	3.798	71.4				
000120	000	0.		6.955	33.339	-2.075	50.	6.955	33.339	-1.727
000121	000	100.		6.956	38.160	-1.379	150.	6.956	40.981	-1.031
000122	000	200.		6.957	42.982	-0.683	250.	6.957	44.535	-0.335
000123	000	300.		6.958	45.803	0.013	400.	6.959	47.805	0.709
000124	000	500.		6.960	49.357	1.405	600.	6.962	50.627	2.101
000125	000	700.		6.965	51.700	2.797	800.	6.968	52.631	3.494
000126	000	900.		6.972	53.451	4.190	1000.	6.975	54.186	4.888
000127	000	1200.		6.983	55.458	6.284	1400.	6.991	56.535	7.681
000128	000	1600.		6.999	57.470	8.963	1800.	7.008	58.294	10.481
000129	000	2000.		7.015	59.033	11.883	2200.	7.022	59.702	13.287
000130	000	2400.		7.031	60.313	14.692	2600.	7.038	60.876	16.099
000131	000	2800.		7.045	61.399	17.507	3000.	7.052	61.885	18.917
000132	000	02	31.9988	0.0						
000133	000	0.		6.958	36.572	-2.075	50.	6.958	36.572	-1.729
000134	000	100.		6.958	41.395	-1.381	150.	6.960	44.216	-1.033
000135	000	200.		6.961	46.218	-0.685	250.	6.992	47.769	-0.337
000136	000	300.		7.023	49.047	0.013	400.	7.196	51.091	0.724
000137	000	500.		7.431	52.722	1.455	600.	7.670	54.098	2.210
000138	000	700.		7.863	55.297	2.986	800.	8.063	56.361	3.786
000139	000	900.		8.212	57.320	4.600	1000.	8.336	58.192	5.427
000140	000	1200.		8.527	59.729	7.114	1400.	8.674	61.055	8.835
000141	000	1600.		8.900	62.222	10.583	1800.	8.916	63.265	12.354
000142	000	2000.		9.029	64.210	14.149	2200.	9.139	65.076	15.966
000143	000	2400.		9.248	65.876	17.804	2600.	9.354	66.620	19.664
000144	000	2800.		9.455	67.317	21.545	3000.	9.551	67.973	23.446
000145	000	H20	18.016	-57.798						

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000146  000      0.0    0.0        0.0      -2.367      50.      3.9805   19.198    -1.974
000147  000    100.     7.961     36.396     -1.561     150.      7.965    39.156    -1.18
000148  000    200.     7.969     41.916      - .784    250.      7.998    43.535    - .384
000149  000    300.     8.027     45.155       .015    400.      8.186    47.483     .825
000150  000    500.     8.415     49.334      1.654    600.      8.676    50.891    2.509
000151  000    700.     8.954     52.249      3.390    800.      9.246    53.464    4.300
000152  000     900.0   9.547     54.570      5.240   1000.0     9.851    55.591    6.209
000153  000    1200.0  10.444     57.440      8.240   1400.0    10.987    59.092   10.384
000154  000    1600.0  11.462     60.591     12.630   1800.0    11.869    61.965   14.964
000155  000    2000.0  12.214     63.234     17.373   2200.0    12.505    64.412   19.846
000156  000    2400.0  12.753     65.511     27.372   2600.0    12.965    66.540   24.945
000157  000    2800.0  13.146     67.508     27.556   3000.0    13.304    68.420   30.201
000158  000  HE        4.003      0.
000159  000       0.          4.968     21.255     -1.461     50.          4.968     21.255     -1.233
000160  000     100.          4.968     24.698     -0.984    150.          4.968     26.128     -0.736
000161  000     200.          4.968     28.142     -0.468    250.          4.968     29.048     -0.239
000162  000     300.          4.968     30.156      0.009    400.          4.968     31.586      0.506
000163  000     500.          4.968     32.694      1.003    600.          4.968     33.600      1.500
000164  000     700.          4.968     34.366      1.996    800.          4.968     35.029      2.493
000165  000     900.          4.968     35.614      2.990   1000.          4.968     36.138      3.487
000166  000    1200.          4.968     37.044      4.481   1400.          4.968     37.809      5.474
000167  000    1600.          4.968     38.473      6.468   1800.          4.968     39.058      7.461
000168  000    2000.          4.968     39.581      8.455   2200.          4.968     40.055      9.449
000169  000    2400.          4.968     40.487     10.442   2600.          4.968     40.885     11.436
000170  000    2800.          4.968     41.253     12.430   3000.          4.968     41.596     13.423
000171  000  M1
000172  000  1.0  1.0  1.0  1.0  1.0  1.0  1.0  0.0  0.0  0.0  1.0  0.0  1.0
000173  000  M2
000174  000  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.5  1.0
000175  000  M3
000176  000  1.0  1.0  1.0  1.0  1.0  1.0  1.0  0.5  0.5  0.6  1.0  0.0  1.0
000177  000  M4
000178  000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  2.0  2.0  2.4  0.0  1.0  0.0
000179  000          C02 GDL REACTION MODEL (AIR-BREATHING)  19 OCT 1976 26 REACTIONS
000180  000  C02110+C02000          =C02100+C02010                12 1.25-13-0.5
000181  000  C02030+C02000          =C02100+C02010                12 1.8 -15-0.5
000182  000  C02030+C02000          =C02020+C02010                12 3.1 -13-0.5
000183  000  C02100+C02000          =C02010+C02010                11 4.0 -13
000184  000  C02020+C02000          =C02010+C02010                12 1.4 -12-0.5
000185  000  C02001+M1             =C02110+M1                    64 1.1 -27-4.8    1484.
000186  000  C02001+M4             =C02110+M4                    64 1.9 -31-5.8    2436.
000187  000  C02001+M1             =C02030+M1                    64 8.1 -31-5.6    1484.
000188  000  C02001+M4             =C02030+M4                    64 1.4 -34-6.6    2436.
000189  000  C02110+M2             =C02030+M2                    62 4.3 -17-1.5
000190  000  C02110+M2             =C02020+M2                    64 4.5 -27-4.2 -   903.
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000191      000   C02110+M2           =C07020+M2          64 8.6 -20-2.5 - 9410.
000192      000   C02110+M2           =C07100+M2          64 8.6 -24-3.8 -  549.
000193      000   C02030+M2           =C07020+M2          64 9.3 -22-3.3 - 1230.
000194      000   C02030+M2           =C07100+M2          64 1.1 -21-3.0 - 1060.
000195      000   C02100+M2           =C07020+M2          62 8.0 -18-1.5
000196      000   C02100+M3           =C02010+M3          64 5.6 -22-3.3 - 1480.
000197      000   C02100+HE           =C07010+HE          14 1.8 -21-3.0    843.
000198      000   C02020+M3           =C02010+M3          64 2.1 -21-3.2 - 1350.
000199      000   C07020+HE           =C07010+HE          14 3.8 -21-3.0    843.
000200      000   C02010+M3           =C02000+M3          64 3.4 -26-4.2   1130.
000201      000   C02010+HE           =C02000+HE          14 9.9 -22-3.0    843.
000202      000   C02001+N2(0)        =C02000+N2(1)       12 8.3 -12 0.5
000203      000   C02010+H20          =C07000+H20         15 3.2 -13           45.5 0.333
000204      000   C02001+H20          =C07030+H20         11 4.0 -13
000205      000   N2(1) +H20          =N2(0) +H20         15 1.1 -10      -   139.0 0.333

END ELT.


@ADD,P DATA


@XQT SEAGULL
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.....................................
.                                   .
.          PROGRAM SEAGULL          .
. SUPERSONIC INVISCID FLOW ANALYSIS .
.    NASA LANGLEY RESEARCH CENTER   .
.         RELEASED 02/01/76         .
.     LAST MODIFICATION 02/25/77    .
.                                   .
.....................................
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TWO DIMENSIONAL FLOW
 CCCC   0000   C A S E  ***
OUTPUT AT EVERY   100 STEPS
GAMMA=   .1200+01 DISTANCE=   .4300+03 TOLERANCE=   .1000+02 SCALE=   .3000+01
ICN= 1  IBN= 1  ISO= 0  ISY= 0  ITY= 0  ITP= 0  IVI= 0
  -.3000+02 DEGREES BREAK IN THE UPPER WALL AT Z=   .1000+01
  -.3000+02 DEGREES BREAK IN THE LOWER WALL AT Z=   .9980+00
```

INITIAL CONDITIONS

TEMPERATURE(DEG. KELVIN)		2.0000000+03
VELOCITY (M/S)		4.5628436+03
PRESSURE(ATM)		2.0000000+00
DENSITY(G/CC)		2.2614246-04
MOLECULAR WT.		1.8554989+01
GAMMA		1.4520176+00
TOTAL ENTHALPY		2.1616025+12
ENTROPY		2.1521133+09
MOLE FRACTION	C02100	3.2200000-03
MOLE FRACTION	C02001	1.6200000-03
MOLE FRACTION	C02000	8.7599999-03
MOLE FRACTION	C02110	1.0830000-02
MOLE FRACTION	C02010	1.0180000-02
MOLE FRACTION	C02020	8.7299999-03
MOLE FRACTION	C02030	3.9299999-03
MOLE FRACTION	N2(0)	3.7432999-01
MOLE FRACTION	N2(1)	7.0239999-02
MOLE FRACTION	02	5.9090000-02
MOLE FRACTION	H20	2.3630000-02
MOLE FRACTION	HE	4.2543999-01

CO2 + OL REACTION MODEL (AIAA-8 BREATHI NO. 1

REACTIONS BEING CONSIDERED

RF=A*EXP(B/RT*M)/T**N

						A	N	B	M
1	C02110+ C02000	= C02100+ C02010	1	2	7.529+10	-.50	.0	.00
2	C02030+ C02000	= C02100+ C02010	1	2	1.084+09	-.50	.0	.00
3	C02030+ C02000	= C02020+ C02010	1	2	1.867+11	-.50	.0	.00
4	C02100+ C02000	= C02010+ C02010	1	1	2.409+11	.00	.0	.00
5	C02020+ C02000	= C02010+ C02010	1	2	8.432+11	-.50	.0	.00
6	C02001+ M1	= C02110+ M1	6	4	6.626-09	-4.80	1484.0	.00
7	C02001+ M4	= C02110+ M4	6	4	1.144-07	-5.80	2436.0	.00
8	C02001+ M1	= C02030+ M1	6	4	4.879-07	-5.60	1484.0	.00
9	C02001+ M4	= C02030+ M4	6	4	8.432-11	-6.60	2436.0	.00
10	C02110+ M2	= C02030+ M2	6	2	2.490+07	-1.50	.0	.00
11	C02110+ M2	= C02020+ M2	6	4	2.710-01	-4.20	-903.0	.00
12	C02110+ M2	= C02020+ M2	6	4	5.300+04	-2.50	-4410.0	.00
13	C02110+ M2	= C02100+ M2	6	4	5.180+00	-3.60	-549.0	.00
14	C02030+ M2	= C02020+ M2	6	4	5.602+02	-3.30	-1230.0	.00
15	C02030+ M2	= C02100+ M2	6	4	6.626+02	-3.00	-1362.0	.00
16	C02100+ M2	= C02020+ M2	6	2	4.819+06	-1.50	.0	.00
17	C02100+ M3	= C02010+ M3	6	4	3.373+02	-3.30	-1480.0	.00
18	C02100+ HE	= C02010+ HE	1	4	1.084+01	-3.00	843.0	.00
19	C02020+ M3	= C02010+ M3	6	4	1.265+03	-3.20	-1350.0	.00
20	C02020+ HE	= C02010+ HE	1	4	2.289+01	-3.00	843.0	.00
21	C02010+ M3	= C02000+ M3	6	4	2.048-02	-4.20	1130.0	.00
22	C02010+ HE	= C02000+ HE	1	4	5.963+02	-3.00	843.0	.00
23	C02001+ N2(D)	= C02000+ N2(1)	1	2	4.999+12	.50	.0	.00
24	C02010+ H20	= C02000+ H20	1	5	1.927+11	.00	45.5	.33
25	C02001+ H20	= C02030+ H20	1	1	2.409+11	.00	.0	.00
26	N2(1) + H20	= N2(0) + H20	1	5	6.626+13	.00	-139.0	.33

CATALYTIC SPECIES BEING CONSIDERED

M1 = 1.00 C02100, 1.00 C02001, 1.00 C07000, 1.00 C02110, 1.00 C02010, 1.00 C02020, 1.00 C02030,
.00 N2(0) , .00 N2(1) , .00 02 , 1.00 H20 , .00 HE ,

M2 = 1.00 C02100, 1.00 C02001, 1.00 C07000, 1.00 C02110, 1.00 C02010, 1.00 C02020, 1.00 C02030,
1.00 N2(0) , 1.00 N2(1) , 1.00 02 , 1.00 H20 , 1.50 HE ,

M3 = 1.00 C02100, 1.00 C02001, 1.00 C07000, 1.00 C02110, 1.00 C02010, 1.00 C02020, 1.00 C02030,
.50 N2(0) , .50 N2(1) , .60 02 , 1.00 H20 , .00 HE ,

M4 = .00 C02100, .00 C02001, .00 C07000, .00 C02110, .00 C02010, .00 C02020, .00 C02030,
2.00 N2(0) , 2.00 N2(1) , 2.40 02 , .00 H20 , 1.00 HE ,

R: D Z: .9950+00 DZ: .0000

LOWER WALL FORCES FR: .0000	FZ: .0000	M: .0000	VFR: .0000	VFZ: .0000	VM: .0000
UPPER WALL FORCES FR: .0000	FZ: .0000	M: .0000	VFR: .0000	VFZ: .0000	VM: .0000
SUM OF FORCES .0000	.0000	.0000	.0000	.0000	.0000

FORCE ON COMPUTATIONAL PLANE: .0000 AREA: .0000
MOMENT ABOUT R AXIS: .0000 MOMENT ABOUT Z AXIS: .0000

I	K	R	P	U	V	T	S	M	THE	RHO	MTOT
0	21	.1100+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	20	.1095+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	19	.1089+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	18	.1084+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	17	.1079+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	16	.1074+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	15	.1068+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	14	.1063+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	13	.1058+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	12	.1053+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	11	.1047+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	10	.1042+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	9	.1037+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	8	.1032+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	7	.1026+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	6	.1021+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	5	.1016+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	4	.1011+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	3	.1005+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01
0	2	.1000+03	.1000+01	.0000	.4820+01	.1000+01	.0000	.4000+01	.0000	.1000+01	.4047+01

MOLE FRACTIONS

PT	R(K)	C02100	C02001	C02000	C02110	C02010	C02020	C02030	MOL WT	GAMMA
21110.00000		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
20109.47368		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
19108.94737		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
18108.42105		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
17107.89474		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
16107.36842		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
15106.84210		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
14106.31579		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
13105.78947		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
12105.26316		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
11104.73684		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
10104.21053		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
9103.68421		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
8103.15789		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
7102.63158		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
6102.10526		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
5101.57895		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
4101.05263		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
3100.52632		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00
2100.00000		3.22000-03	1.62000-03	8.76000-03	1.08300-02	1.01800-02	8.73000-03	3.93000-03	1.00000+00	1.45202+00

MOLE FRACTIONS

PT	P(N)	N2(0)	N2(1)	O2	H2O	HE		
21110.00000	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
20109.47368	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
19108.94737	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
18108.42105	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
17107.89474	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
16107.36842	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
15106.84210	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
14106.31579	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
13105.78947	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
12105.26316	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
11104.73684	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
10104.21053	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
9103.68421	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
8103.15789	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
7102.63158	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
6102.10526	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
5101.57895	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
4101.05263	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
3100.52632	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00
2100.00000	3.74330-01	7.02400-02	5.90900-02	2.36300-02	4.25440-01	1.00000+00	1.45202+00

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15. Supplementary Notes

Langley Technical Monitor: Manuel D. Salas

Final Report

16. Abstract

A two-dimensional multiple shock nozzle code (SEAGULL) has been extended to include the effects of finite rate chemistry. The basic code that treats multiple shocks and contact surfaces was fully coupled with a generalized finite rate chemistry and vibrational energy exchange package. The modified code retains all of the original SEAGULL features plus the capability to treat chemical and vibrational nonequilibrium reactions. Any chemical and/or vibrational energy exchange mechanism can be handled as long as thermodynamic data and rate constants are available for all participating species.

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